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Ma

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(54) **ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES**

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(51) **Int. Cl.**

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H01L 51/50	(2006.01)
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CPC ***C07D 495/04*** (2013.01); ***C07D 495/14*** (2013.01); ***C07F 7/0812*** (2013.01); ***H01L 51/0054*** (2013.01); ***H01L 51/0071*** (2013.01); ***H01L 51/0072*** (2013.01); ***H01L 51/0074*** (2013.01); ***H01L 51/0094*** (2013.01); *H01L 51/0085* (2013.01); *H01L 51/5012* (2013.01); *H01L 51/5016* (2013.01); *H01L 51/5096* (2013.01)

(58) **Field of Classification Search**

CPC C07D 495/04; C07D 495/14

See application file for complete search history.

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(57) **ABSTRACT**

Novel heterocyclic materials are disclosed. The materials contain a fused tetracyclic structure that can improve the properties of OLED devices when the novel heterocyclic materials are incorporated into such devices.

20 Claims, 3 Drawing Sheets

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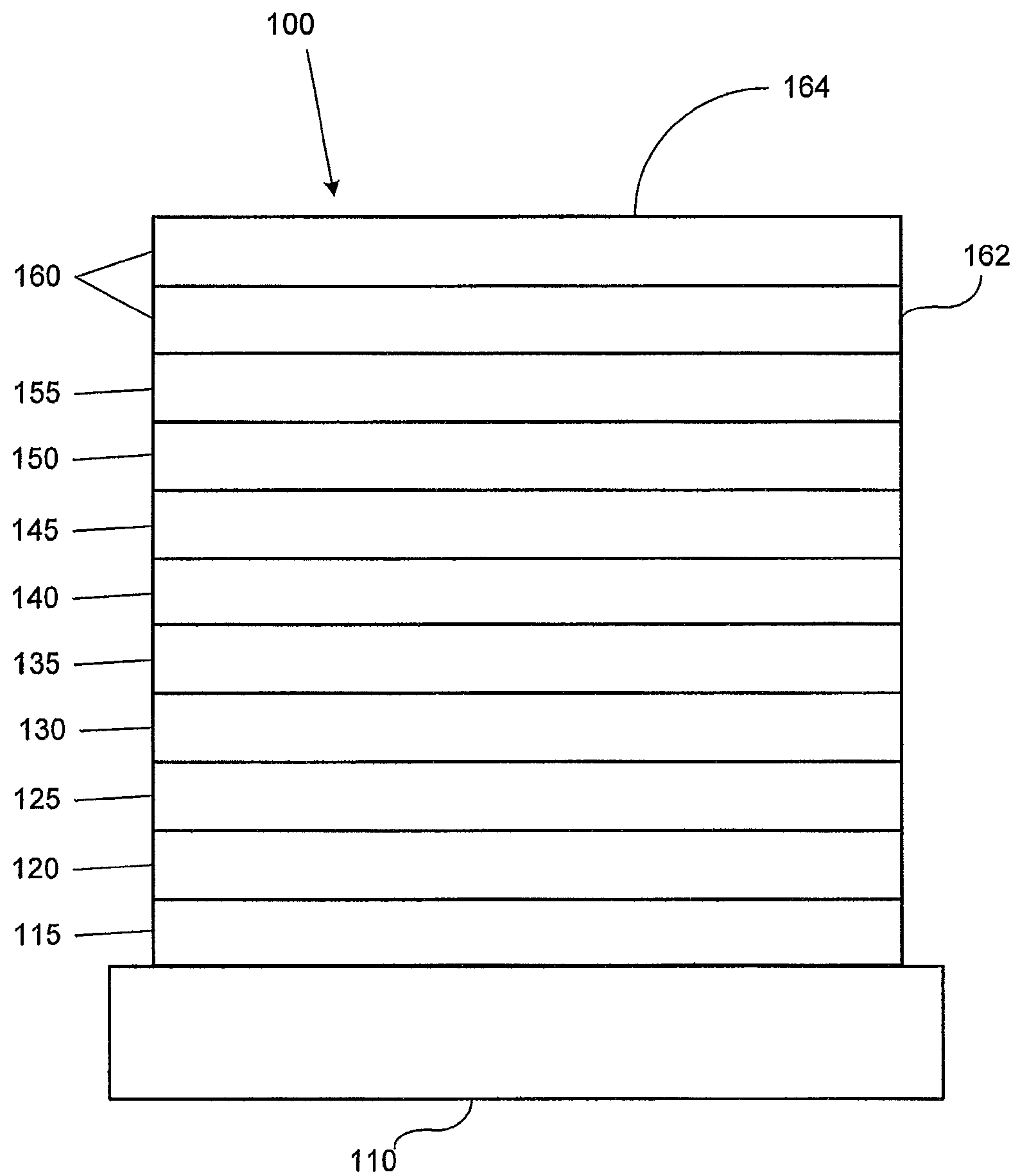


FIGURE 1

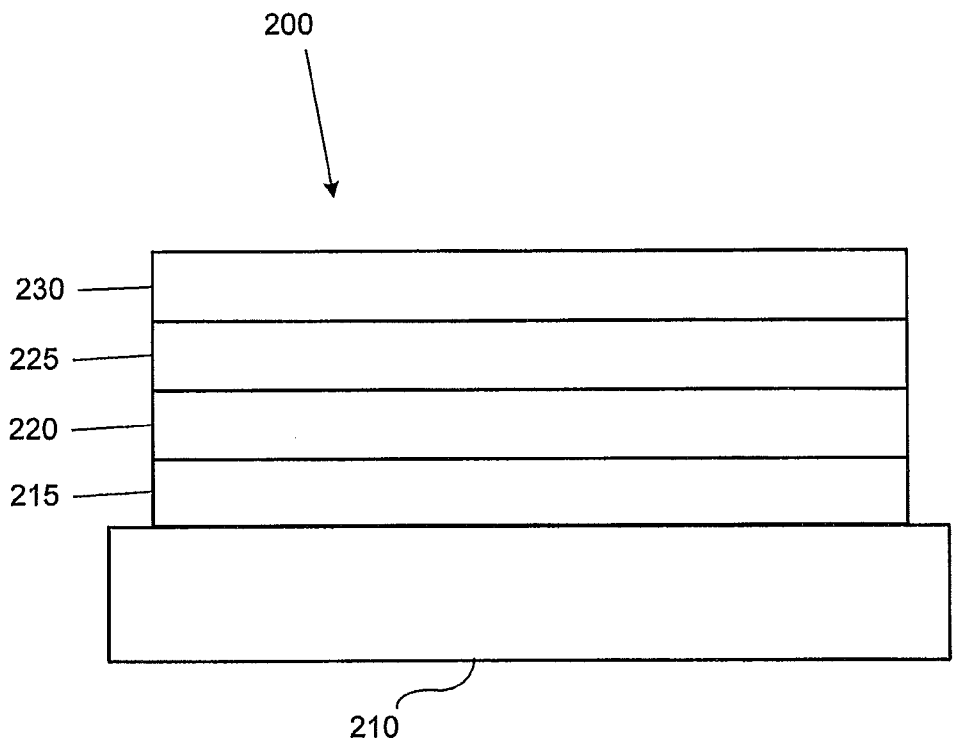
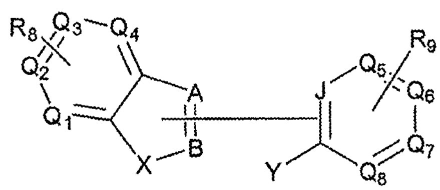


FIGURE 2



Formula I

FIGURE 3

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

CROSS-REFERENCE TO RELATED APPLICATIONS

This application is a divisional application of U.S. patent application Ser. No. 13/347,305, filed Jan. 10, 2012, the entire content of which is incorporated herein by reference.

PARTIES TO A JOINT RESEARCH AGREEMENT

The claimed invention was made by, on behalf of, and/or in connection with one or more of the following parties to a joint university corporation research agreement: The Regents of the University of Michigan, Princeton University, University of Southern California, and Universal Display Corporation. The agreement was in effect on and before the date the claimed invention was made, and the claimed invention was made as a result of activities undertaken within the scope of the agreement.

FIELD OF THE INVENTION

The present invention relates to novel heterocyclic host materials suitable for incorporation into OLED devices. Devices incorporating the novel host materials described herein are expected to have improved properties such as increased efficiency and stability.

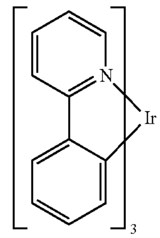
BACKGROUND

Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition, the inherent properties of organic materials, such as their flexibility, may make them well suited for particular applications such as fabrication on a flexible substrate. Examples of organic opto-electronic devices include organic light emitting devices (OLEDs), organic phototransistors, organic photovoltaic cells, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials. For example, the wavelength at which an organic emissive layer emits light may generally be readily tuned with appropriate dopants.

OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting. Several OLED materials and configurations are described in U.S. Pat. Nos. 5,844,363, 6,303,238, and 5,707,745, which are incorporated herein by reference in their entirety.

One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as "saturated" colors. In particular, these standards call for saturated red, green, and blue pixels. Color may be measured using CIE coordinates, which are well known to the art.

One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted $Ir(ppy)_3$, which has the following structure:



In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

As used herein, the term "organic" includes polymeric materials as well as small molecule organic materials that may be used to fabricate organic opto-electronic devices. "Small molecule" refers to any organic material that is not a polymer, and "small molecules" may actually be quite large. Small molecules may include repeat units in some circumstances. For example, using a long chain alkyl group as a substituent does not remove a molecule from the "small molecule" class. Small molecules may also be incorporated into polymers, for example as a pendent group on a polymer backbone or as a part of the backbone. Small molecules may also serve as the core moiety of a dendrimer, which consists of a series of chemical shells built on the core moiety. The core moiety of a dendrimer may be a fluorescent or phosphorescent small molecule emitter. A dendrimer may be a "small molecule," and it is believed that all dendrimers currently used in the field of OLEDs are small molecules.

As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer. For example, a cathode may be described as "disposed over" an anode, even though there are various organic layers in between.

As used herein, "solution processible" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

A ligand may be referred to as "photoactive" when it is believed that the ligand directly contributes to the photoactive properties of an emissive material. A ligand may be referred to as "ancillary" when it is believed that the ligand does not contribute to the photoactive properties of an emissive material, although an ancillary ligand may alter the properties of a photoactive ligand.

As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conventional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than the HOMO energy level of the same material. A "higher"

HOMO or LUMO energy level appears closer to the top of such a diagram than a "lower" HOMO or LUMO energy level.

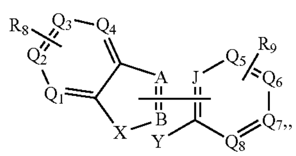
As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum level, this means that a "higher" work function is more negative. On a conventional energy level diagram, with the vacuum level at the top, a "higher" work function is illustrated as further away from the vacuum level in the downward direction. Thus, the definitions of HOMO and LUMO energy levels follow a different convention than work functions.

More details on OLEDs, and the definitions described above, can be found in U.S. Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

SUMMARY OF THE INVENTION

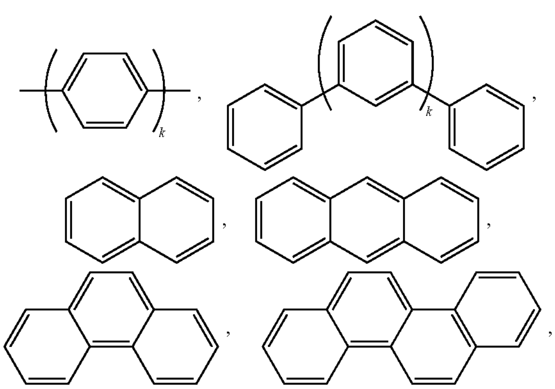
In one aspect a compound having the formula:

Formula I



is provided. In the compound of Formula I, Q_1 to Q_8 are independently selected from CH and N, and wherein Q_1 to Q_8 may be further substituted. A is directly bonded to J and B is directly bonded to Y, or wherein A is directly bonded to Y and B is directly bonded to J. A, B, and J are carbon atoms. X and Y are independently selected from the group consisting of O, S, and Se. R_8 and R_9 independently represent mono, di, tri, tetra substitution, or no substitution. R_8 and R_9 are independently selected from the group consisting of deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof, and at least one of R_8 and R_9 is not hydrogen or deuterium.

In one aspect, at least one of R_8 and R_9 is independently selected from the group consisting of:



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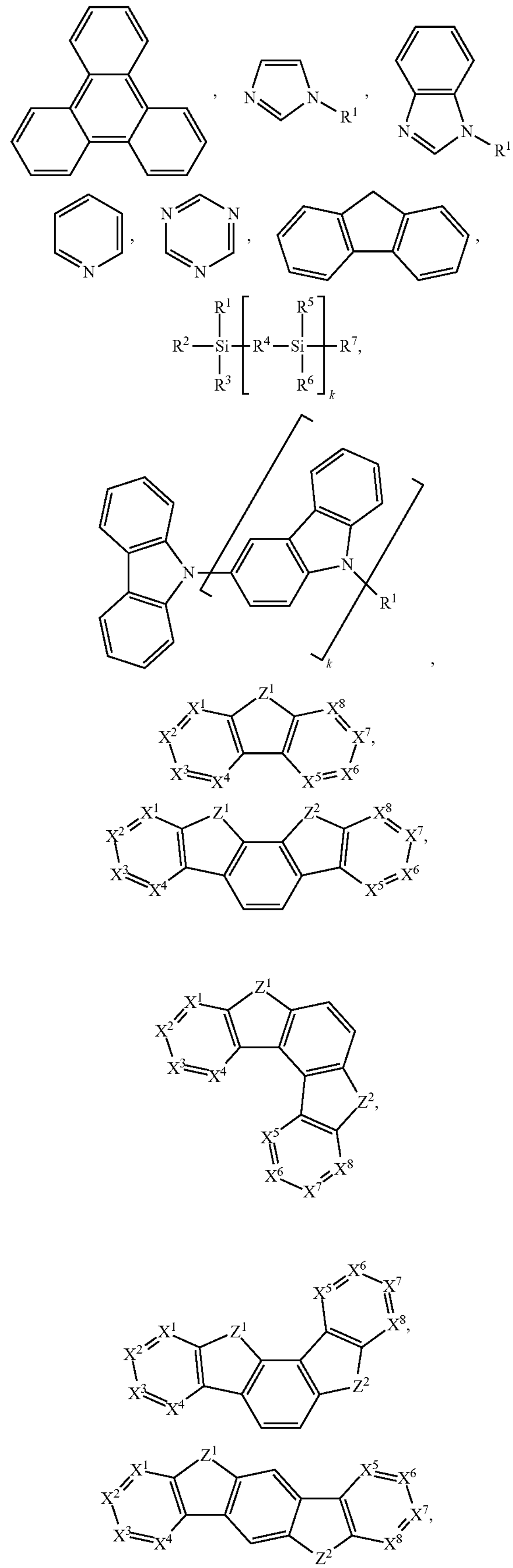

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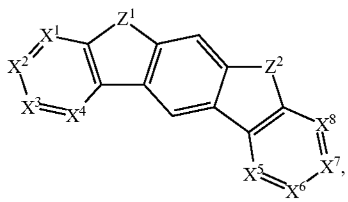
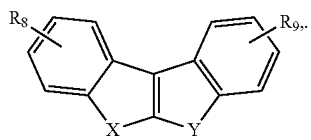


wherein R^1 to R^7 is independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof k is an integer from 0 to 20, X^1 to X^8 are independently selected from C, CH, and N, Z^1 and Z^2 is selected from NR^1, O, or S; and R_8 and R_9 may be further substituted.

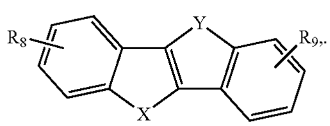
In one aspect, the compound has the formula:

Formula II



In one aspect, the compound has the formula:

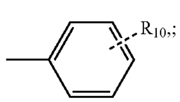
Formula III



In one aspect, one of Q_1 to Q_8 is N.

In one aspect, at least one of R_8 and R_9 has the formula:

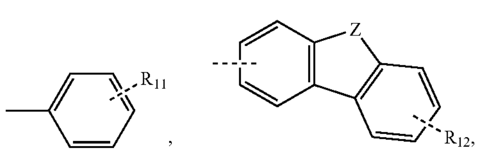
Formula IV



wherein R_{10} represents mono, di, tri, tetra substitution, or no substitution and

wherein R_{10} is selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

In one aspect, R_{10} represents mono-substitution and is selected from the group consisting of:



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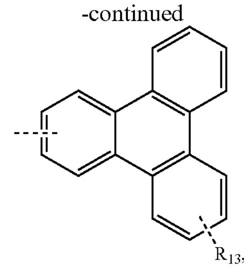
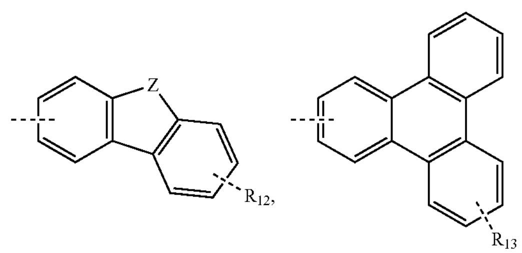


SiRR'R" and combinations thereof. Z is selected from the group consisting of NR, S, O, and Se. R_{11}, R_{12}, and R_{13} represents mono, di, tri, tetra substitution, or no substitution. R, R', R", R_{11}, R_{12}, and R_{13} are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

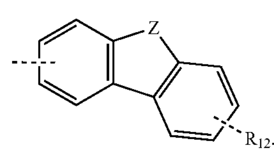
In one aspect, at least one of R_8 and R_9 is independently selected from the group consisting of:



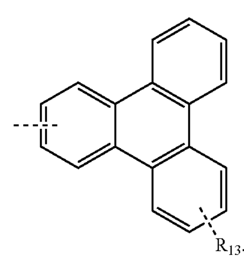
SiRR'R" and combinations thereof. Z is selected from the group consisting of NR, S, O, and Se. R_{12} and R_{13} represents mono, di, tri, tetra substitution, or no substitution, and R, R', R", R_{12}, and R_{13} are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

In one aspect, X and Y are S.

In one aspect, at least one of R_8 and R_9 is



In one aspect, at least one of R_8 and R_9 is

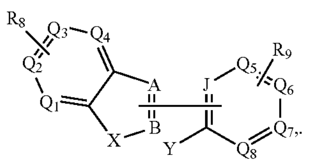


In one aspect, at least one of R_8 and R_9 is SiRR'R". In another aspect, R_8 is ortho or para to X, and wherein R_9 is ortho or para to Y. In one aspect, R_8 is ortho or para to X, and wherein R_9 is ortho or para to Y. In one aspect, R_8 is hydrogen or deuterium.

In one aspect, the compound is selected from the group consisting of Compound 1-Compound 52.

In one aspect, a first device comprising an organic light emitting device, further comprising an anode, a cathode, and an organic layer, disposed between the anode and the cathode, comprising a compound having the formula:

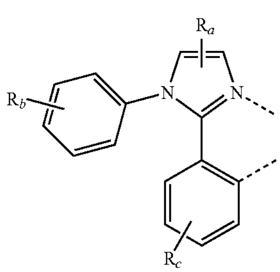
Formula I

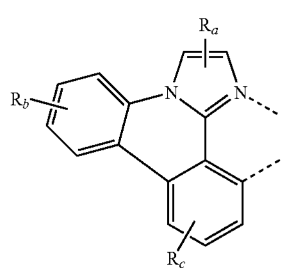


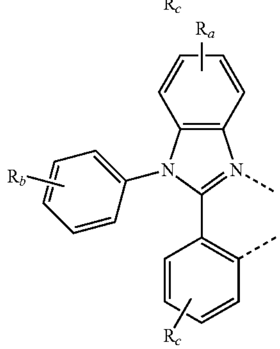
In the compound of Formula I, Q_1 to Q_8 are independently selected from CH and N, and wherein Q_1 to Q_8 may be further substituted. A is directly bonded to J and B is directly bonded to Y, or wherein A is directly bonded to Y and B is directly bonded to J. A, B, and J are carbon atoms. X and Y are independently selected from the group consisting of O, S, and Se. R_8 and R_9 independently represent mono, di, tri, tetra substitution, or no substitution. R_8 and R_9 are independently selected from the group consisting of deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof, and at least one of R_8 and R_9 is not hydrogen or deuterium.

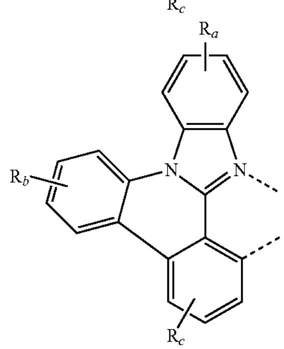
In one aspect, the organic layer is an emissive layer and the compound of Formula I is a host. In one aspect, the organic layer further comprises an emissive dopant.

In one aspect, the emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:









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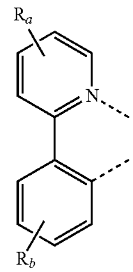

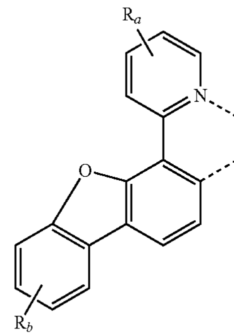

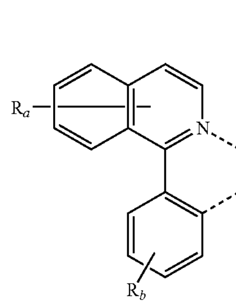

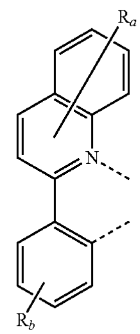

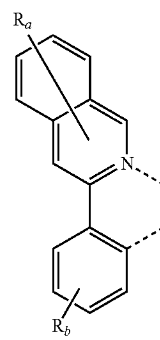

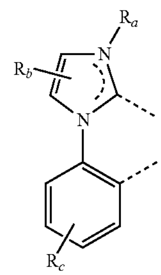

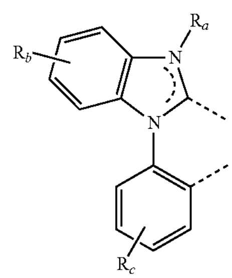

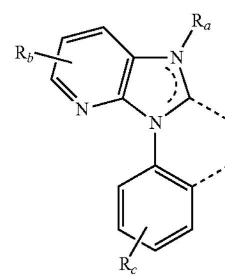

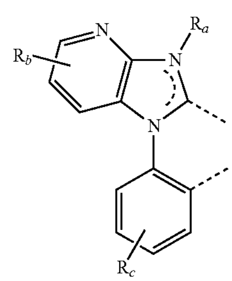

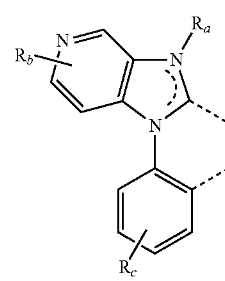

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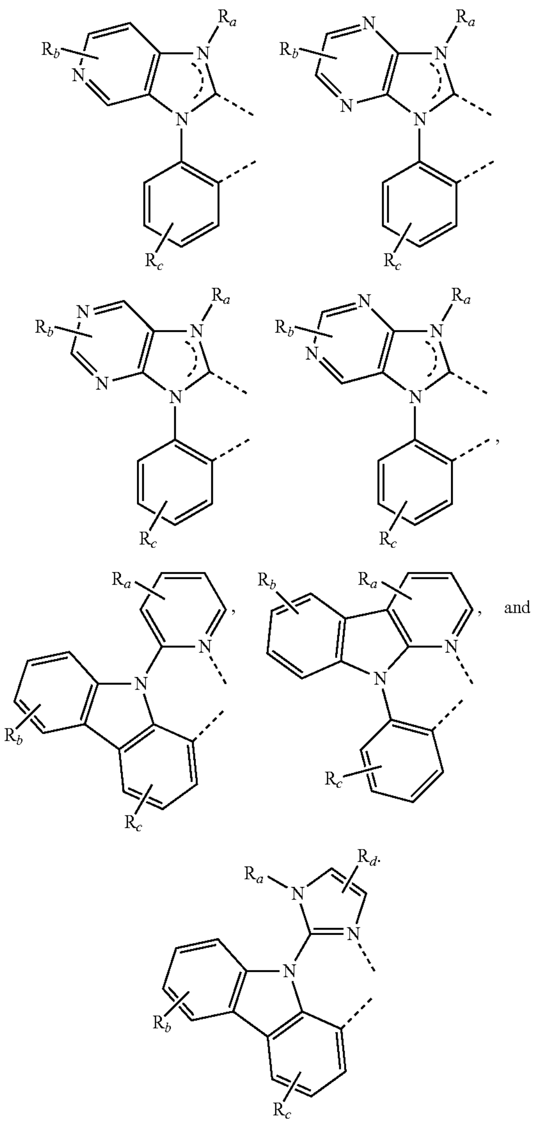


R_a, R_b, and R_c may represent mono, di, tri or tetra substitutions, or no substitution, and R_a, R_b, and R_c are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof. Two adjacent substituents of R_a, R_b, and R_c are optionally joined to form a fused ring or form a multidentate ligand.

In one aspect, the device further comprises a second organic layer that is a non-emissive layer and the compound having Formula I is a material in the second organic layer.

In one aspect, the second organic layer is a blocking layer and the compound having Formula I is a blocking material in the second organic layer.

In one aspect, the first device is a consumer product. In one aspect, the first device is an organic light-emitting device. In one aspect, the first device comprises a lighting panel.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. **1** shows an organic light emitting device.

FIG. **2** shows an inverted organic light emitting device that does not have a separate electron transport layer.

FIG. **3** shows a compound of Formula I.

DETAILED DESCRIPTION

Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an electron and hole localize on the same molecule, an "exciton," which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized on an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable.

The initial OLEDs used emissive molecules that emitted light from their singlet states ("fluorescence") as disclosed, for example, in U.S. Pat. No. 4,769,292, which is incorporated by reference in its entirety. Fluorescent emission generally occurs in a time frame of less than 10 nanoseconds.

More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), which are incorporated by reference in their entireties. Phosphorescence is described in more detail in U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

FIG. **1** shows an organic light emitting device **100**. The figures are not necessarily drawn to scale. Device **100** may include a substrate **110**, an anode **115**, a hole injection layer **120**, a hole transport layer **125**, an electron blocking layer **130**, an emissive layer **135**, a hole blocking layer **140**, an electron transport layer **145**, an electron injection layer **150**, a protective layer **155**, and a cathode **160**. Cathode **160** is a compound cathode having a first conductive layer **162** and a second conductive layer **164**. Device **100** may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F.sub.4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

FIG. **2** shows an inverted OLED **200**. The device includes a substrate **210**, a cathode **215**, an emissive layer **220**, a hole transport layer **225**, and an anode **230**. Device **200** may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device **200** has cathode **215** disposed under anode **230**, device **200** may be referred to as an "inverted" OLED. Materials similar to those described with respect to device **100** may be used in the corresponding layers of device **200**. FIG. **2** provides one example of how some layers may be omitted from the structure of device **100**.

The simple layered structure illustrated in FIGS. **1** and **2** is provided by way of non-limiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device **200**, hole transport layer **225** transports holes and injects holes into emissive layer **220**, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an "organic layer" disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. **1** and **2**.

Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. **1** and **2**. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. patent application Ser. No. 10/233,470, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink jet and OVJD. Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processibility than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

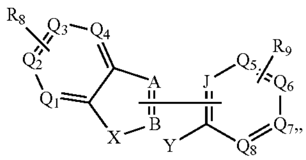
Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent displays, flexible displays, laser printers, telephones, cell phones, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, vehicles, a large area wall, theater or stadium screen, or a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C.).

The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures.

The terms halo, halogen, alkyl, cycloalkyl, alkenyl, alkynyl, arylkyl, heterocyclic group, aryl, aromatic group, and heteroaryl are known to the art, and are defined in U.S. Pat. No. 7,279,704 at cols. 31-32, which are incorporated herein by reference.

In one embodiment a compound having the formula:

Formula I



is provided. In the compound of Formula I, Q_1 to Q_8 are independently selected from CH and N, and wherein Q_1 to Q_8 may be further substituted. A is directly bonded to J and B is directly bonded to Y, or wherein A is directly bonded to Y and B is directly bonded to J. A, B, and J are carbon atoms. X and Y are independently selected from the group consisting of O, S, and Se. R_8 and R_9 independently represent mono, di, tri, tetra substitution, or no substitution. R_8 and R_9 are independently selected from the group consisting of deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof, and at least one of R_8 and R_9 is not hydrogen or deuterium.

DBT (dibenzothiophene) containing hosts show significant device performance improvement with respect to device stability and efficiency when such compounds are incorporated into\phosphorescent OLED devices, see, e.g. WO 2009021126. Compounds of Formula I have an additional ring fused into the ring system, making them tetracyclic compounds, whereas DBT and DBF (dibenzofuran) are tricyclic ring systems. However, based on DFT calculations, the triplet energy of molecules containing the core structure of compounds of Formula I show relatively high energy, especially when X and Y are heteroatoms and on the same side, i.e. Compounds of Formula II. Molecules containing the core in compounds of Formula II have higher calculated triplet energy than molecules containing the core of compounds of Formula III. These results are summarized in Table 1.

TABLE 1

Calculated Energy Levels foe Molecules Containing the Core of Compounds of Formula I[a]

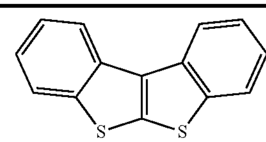
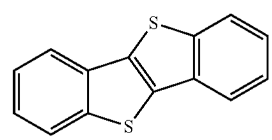
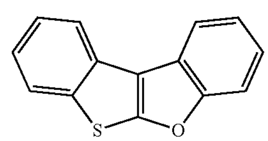
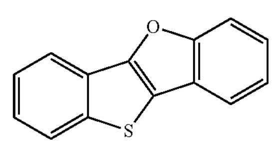
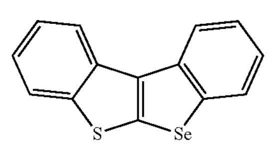
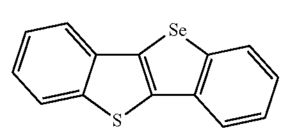
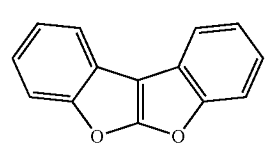
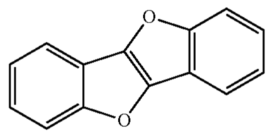
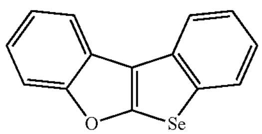
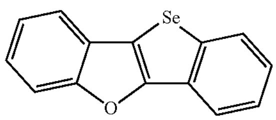
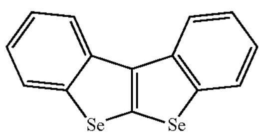
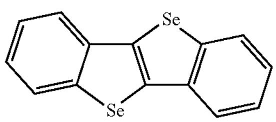
Molecule #	Structure	HOMO (ev)	LUMO (ev)	HOMO − LUMO (ev)	Dipole (Debye)	Calc. T1 (nm)
1.		−5.60	−0.86	−4.74	1.30	418
2.		−5.58	−1.26	−4.32	0.00	462
3.		−5.57	−0.61	−4.96	1.19	394
4.		−5.55	−1.17	−4.38	0.24	456
5.		−5.55	−0.88	−4.67	1.09	423
6.		−5.52	−1.28	−4.24	0.16	467
7.		−5.55	−0.38	−5.17	1.14	369

TABLE 1-continued

Calculated Energy Levels foe Molecules Containing the Core of Compounds of Formula I[a]

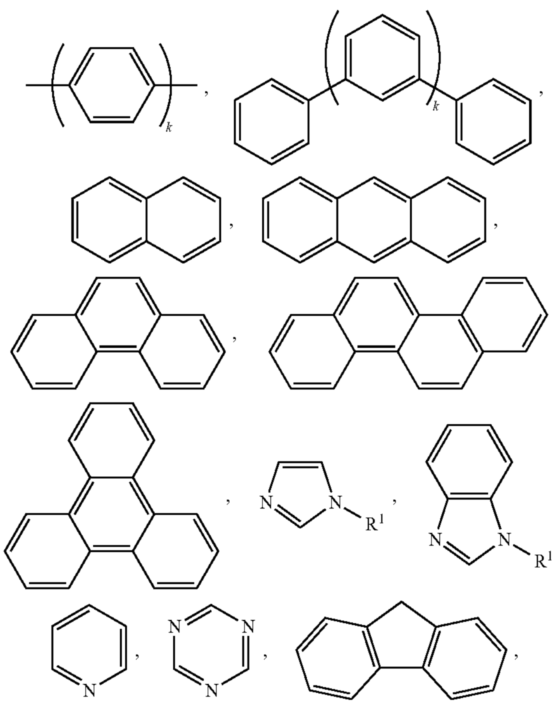
Molecule #	Structure	HOMO (ev)	LUMO (ev)	HOMO − LUMO (ev)	Dipole (Debye)	Calc. T1 (nm)
8.		−5.52	−1.10	−4.42	0.00	451
9.		−5.51	−0.64	−4.87	1.00	401
10.		−5.50	−1.18	−4.32	0.21	461
11.		−5.51	−0.90	−4.61	0.88	428
12.		−5.47	−1.30	−4.17	0.00	473

[a]Calculation is based on DFT/B3LYP/6-31g(d) optimized geometry

b. The basis set used for Al, Bi, Zr, Ga, Ge, Y, Sc, Y, Ru, Zn, W, Mo, Os, Pt, Ir and Hf is cep-31g, the basis set used for all other elements is 6-31g(d)

From Table 1, we can see that the calculated triplet energy of molecule 1 and 7 are 418 nm and 369 nm, respectively. The experimental T1 of DBT is 415 nm and the experimental T1 of DBF is 417 nm. These results indicate that molecules containing the core of compounds of Formula I have potentially even higher triplet energy than DBT or DBF even with more fused cyclic rings and heteroatoms. These properties may be beneficial when compounds of Formula I are incorporated into OLED devices. Without being bound by theory, it is believed that compounds of Formula I would have better charge transport and charge stabilization properties as a result of the extended conjugation in compounds of Formula I in comparison to DBT- or DBF-type compounds. For example, the measured experimental T1 of Compound 3 was about 470 nm as predicted, which is very similar to the T1 (472 nm) of its DBT analog. Typically, increasing conjugation in host molecules results in the decrease of T1. However, it has unexpectedly been found that compounds of Formula I, which have increased conjugation in comparison to a DBT or DBF core actually maintain their T1 or in some instances have an even higher T1.

In one embodiment, at least one of R_8 and R_9 is independently selected from the group consisting of:



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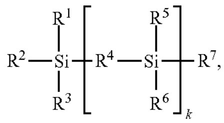
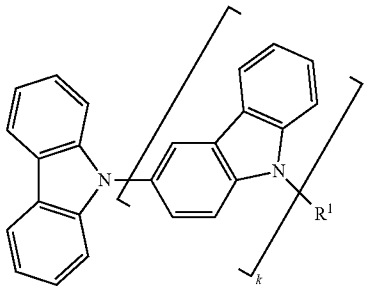
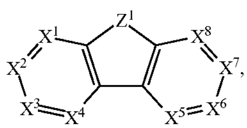
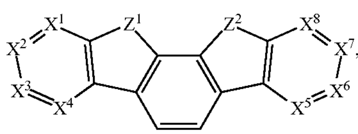
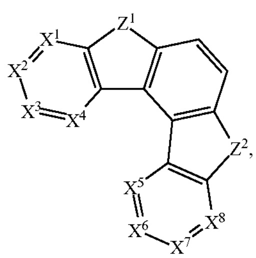
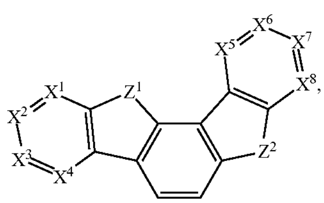


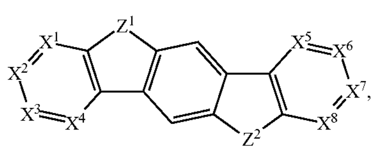


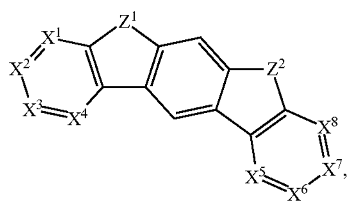








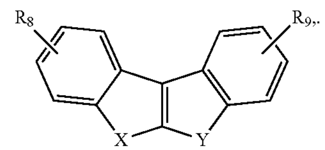




wherein R^1 to R^7 is independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof k is an integer from 0 to 20, X^1 to X^8 are independently selected from C, CH, and N, Z^1 and Z^2 is selected from NR^1, O, or S; and R_8 and R_9 may be further substituted.

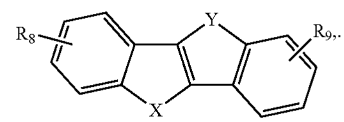
In one embodiment, the compound has the formula:

Formula II



In one embodiment, the compound has the formula:

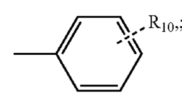
Formula III



In one embodiment, one of Q_1 to Q_8 is N.

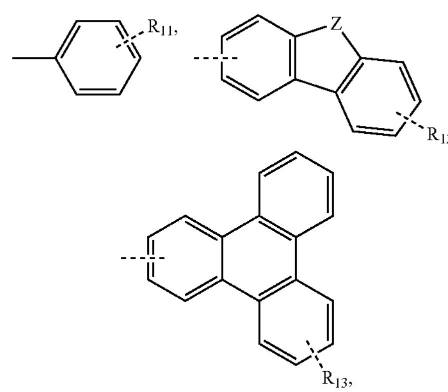
In one embodiment, at least one of R_8 and R_9 has the formula:

Formula IV



wherein R_{10} represents mono, di, tri, tetra substitution, or no substitution and wherein R_{10} is selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

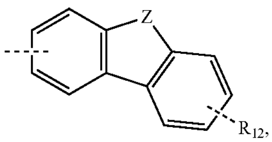
In one embodiment, R_{10} represents mono-substitution and is selected from the group consisting of:

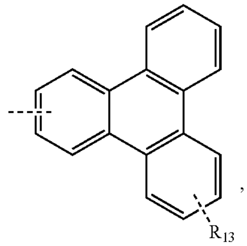


SiRR'R" and combinations thereof. Z is selected from the group consisting of NR, S, O, and Se. R_{11}, R_{12}, and R_{13} represents mono, di, tri, tetra substitution, or no substitution. R, R', R", R_{11}, R_{12}, and R_{13} are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

When Z is N—R, R_8, R_9, or R_{10} can connect to other portions of a compound of Formula I through the N or through a substituent bonded to the N, i.e. the R group attached to the N.

In one embodiment, at least one of R_8 and R_9 is independently selected from the group consisting of:

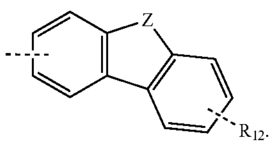




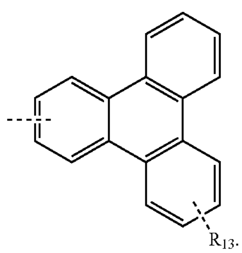
SiRR'R" and combinations thereof. Z is selected from the group consisting of NR, S, O, and Se. R_{12} and R_{13} represents mono, di, tri, tetra substitution, or no substitution, and R, R', R", R_{12}, and R_{13} are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

In one embodiment, X and Y are S.

In one embodiment, at least one of R_8 and R_9 is



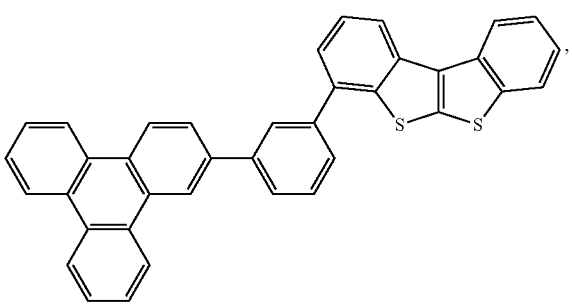
In one embodiment, at least one of R_8 and R_9 is



In one embodiment, at least one of R_8 and R_9 is SiRR'R". In another embodiment, R_8 is ortho or para to X, and wherein R_9 is ortho or para to Y. In one embodiment, R_8 is ortho or para to X, and wherein R_9 is ortho or para to Y. In one embodiment, R_8 is hydrogen or deuterium.

In one embodiment, the compound is selected from the group consisting of:

Compound 1



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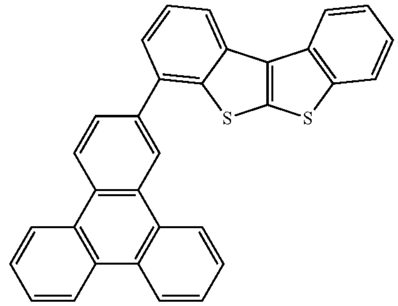
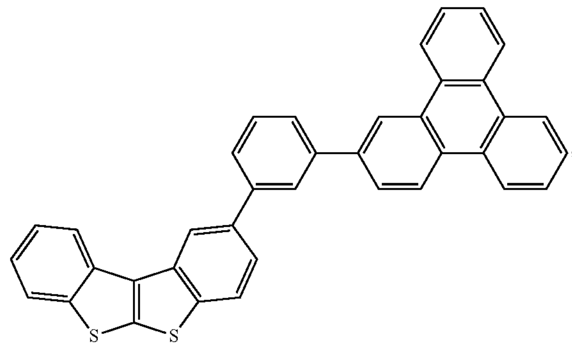
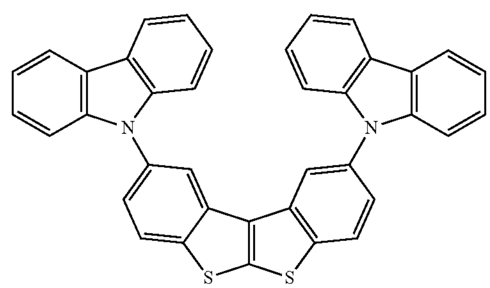
Compound 2



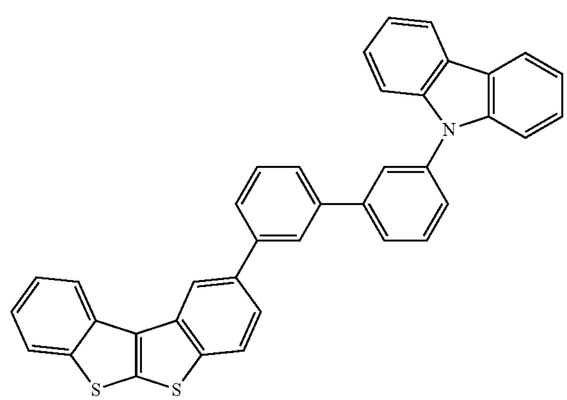
Compound 3



Compound 4



Compound 5



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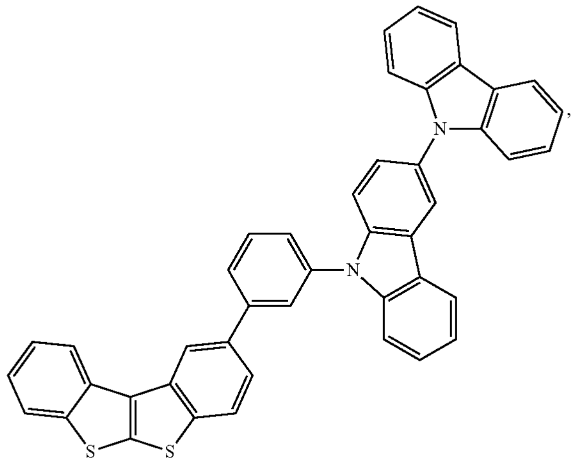
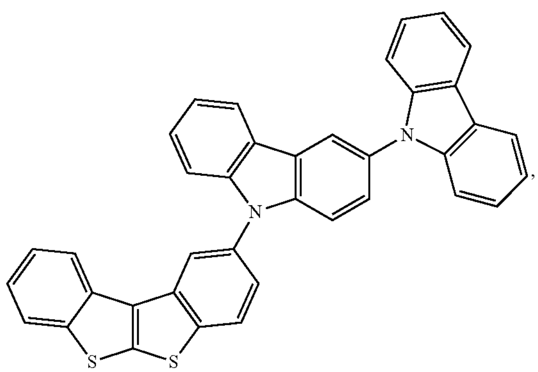
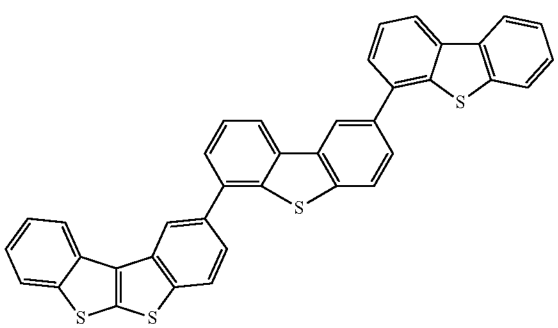
Compound 6



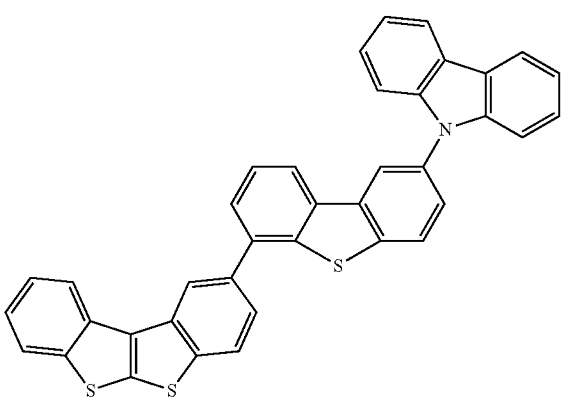
Compound 7



Compound 8



Compound 9



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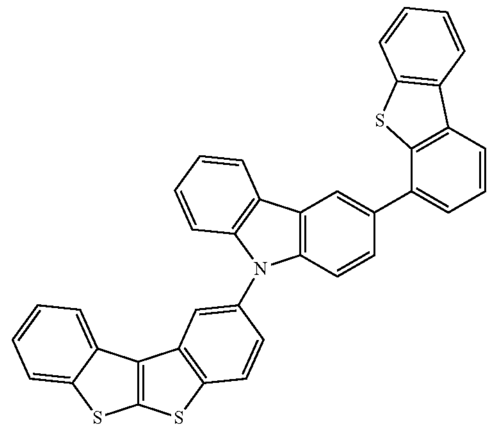
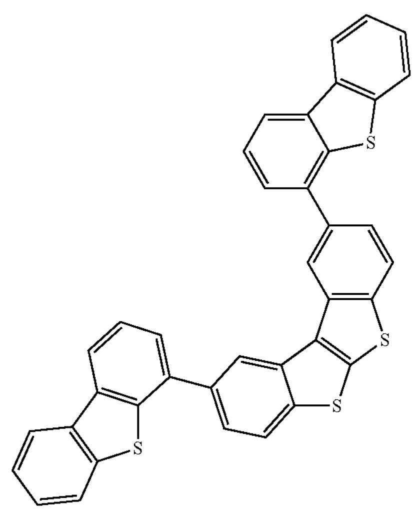
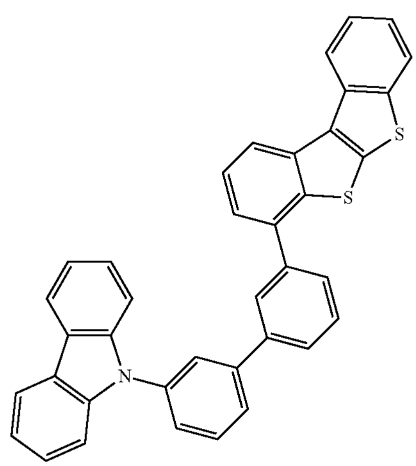
Compound 10



Compound 11



Compound 12



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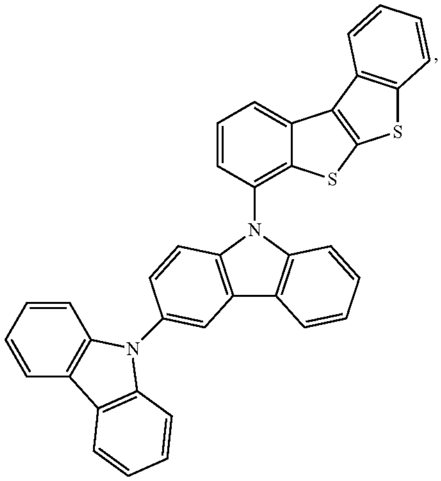
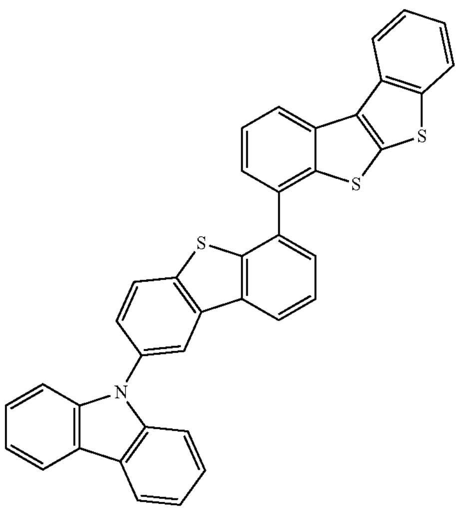
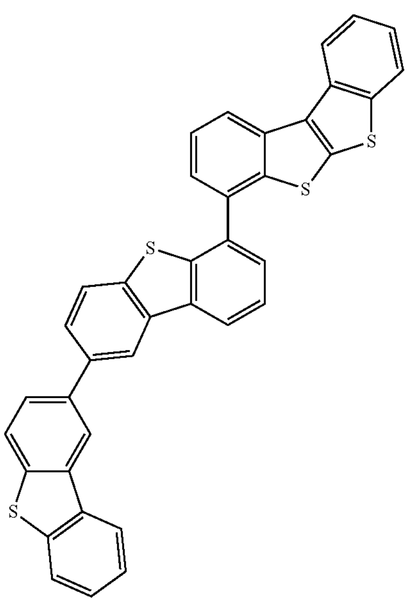
Compound 13



Compound 14



Compound 15



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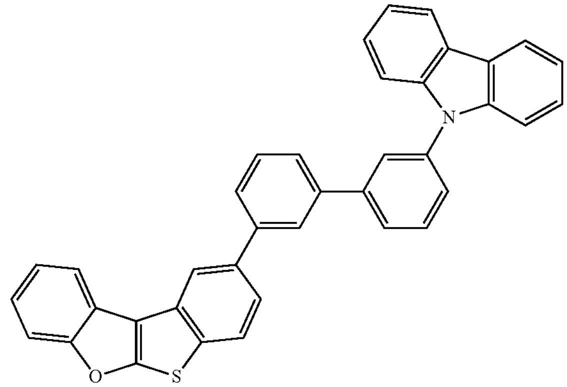
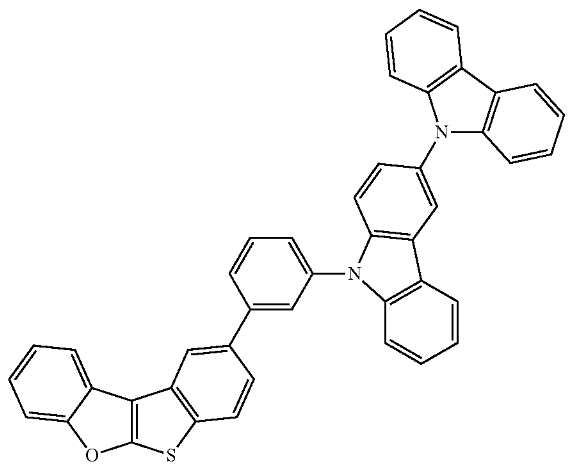
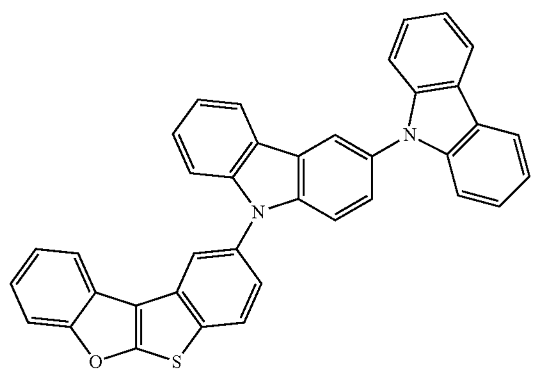
Compound 16



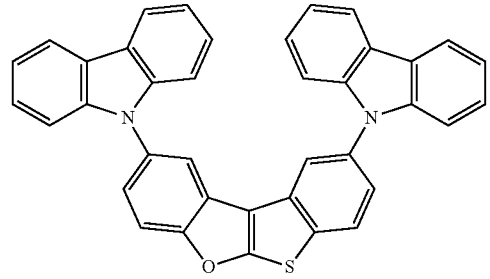
Compound 17



Compound 18



Compound 19



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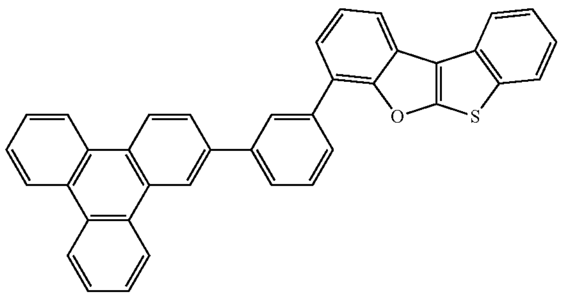
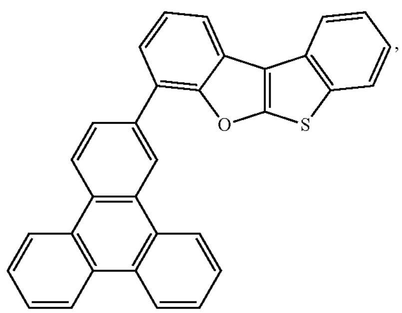
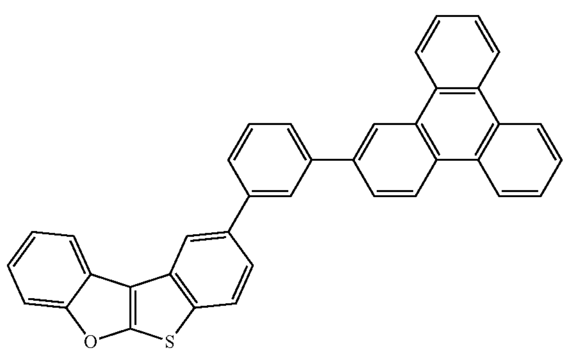
Compound 20



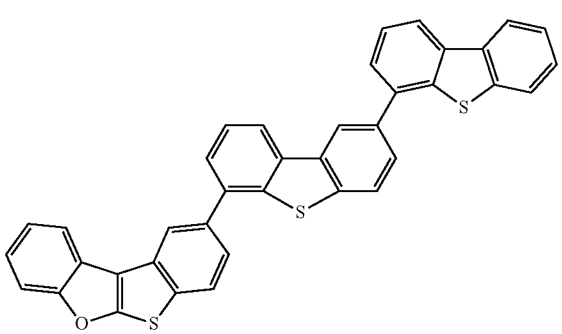
Compound 21



Compound 22



Compound 23



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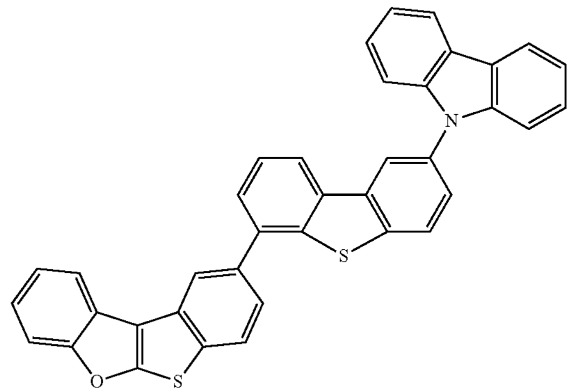
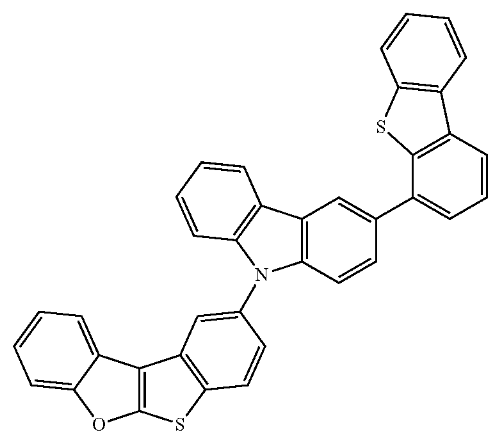
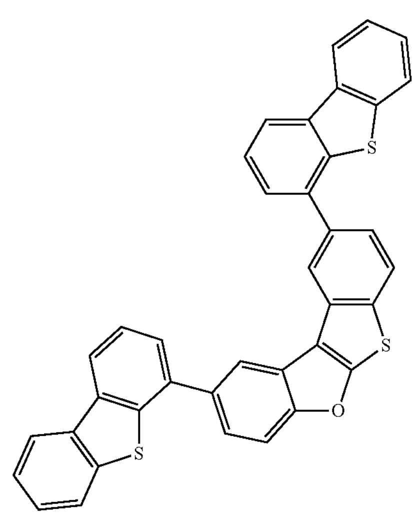
Compound 24



Compound 25



Compound 26



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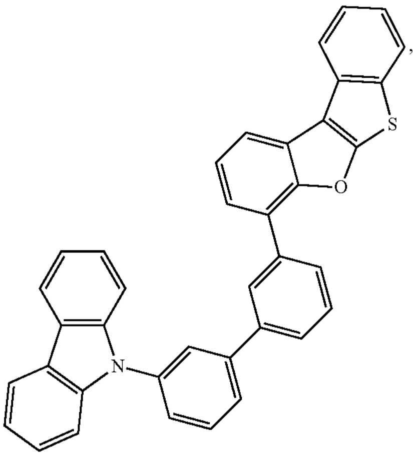
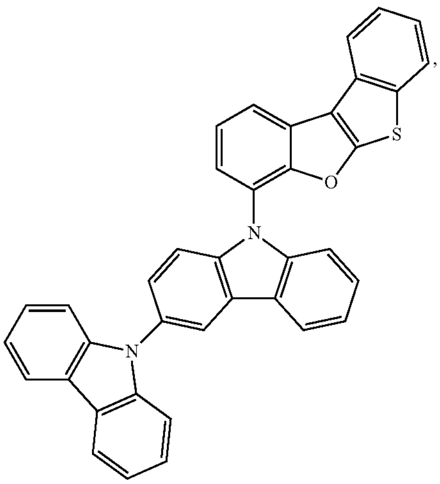
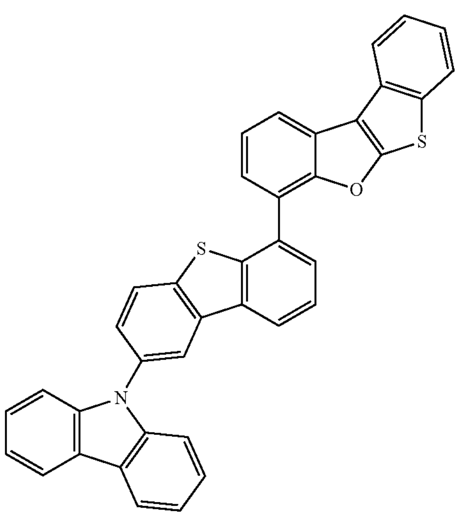
Compound 27



Compound 28

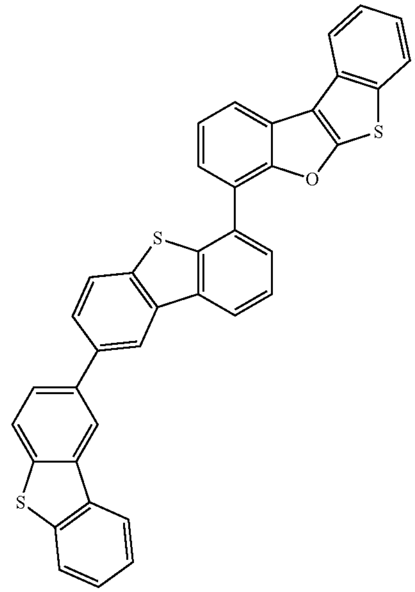


Compound 29

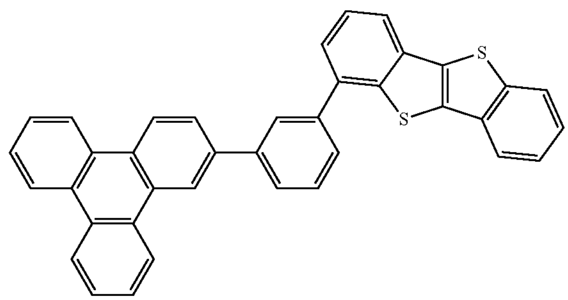


-continued

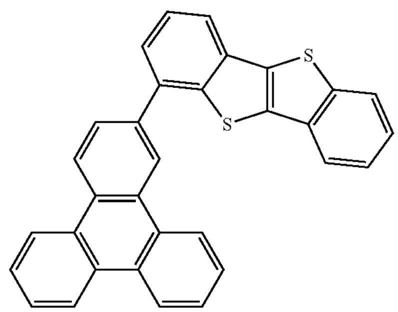
Compound 30



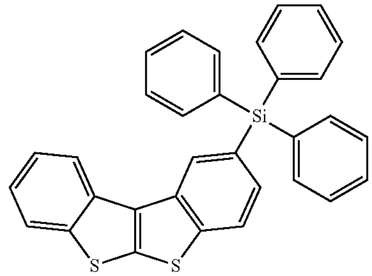
Compound 31



Compound 32



Compound 33



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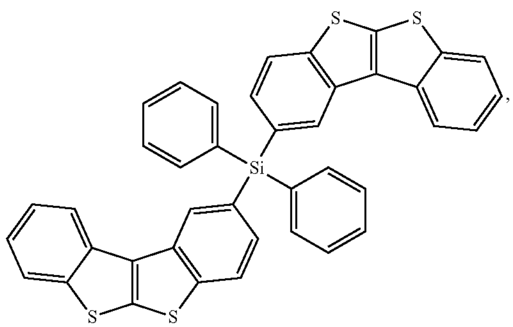
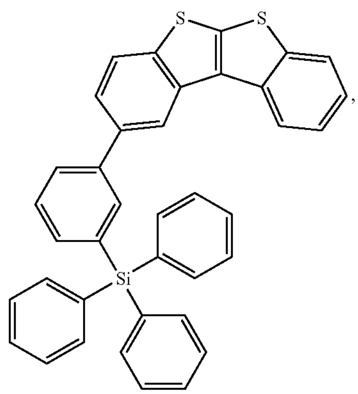
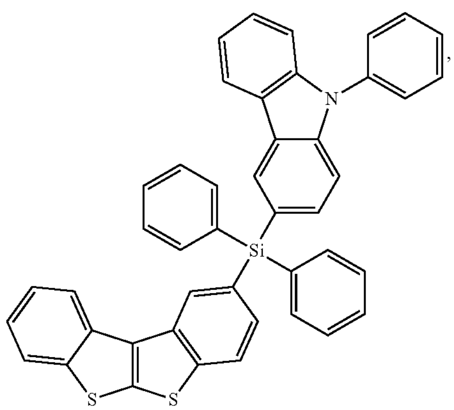
Compound 34



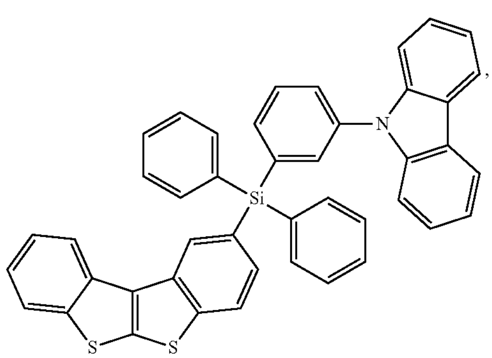
Compound 35



Compound 36

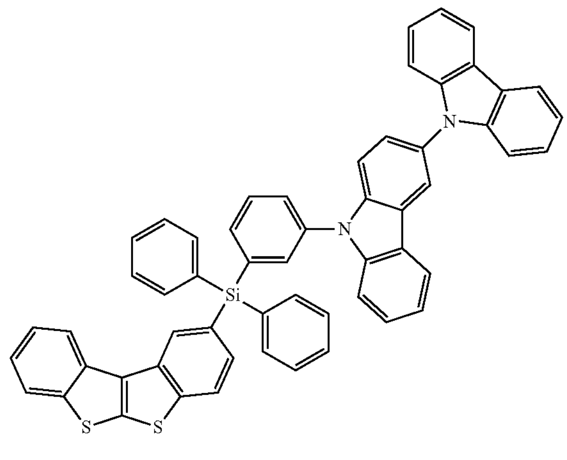


Compound 37

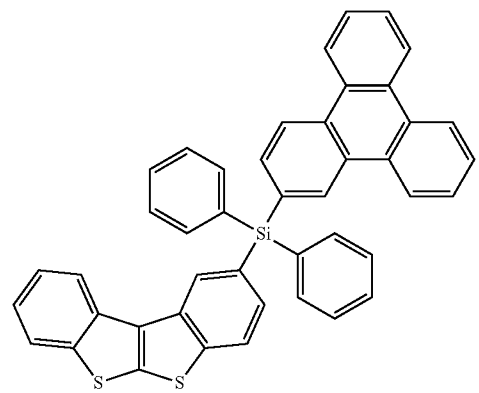


-continued

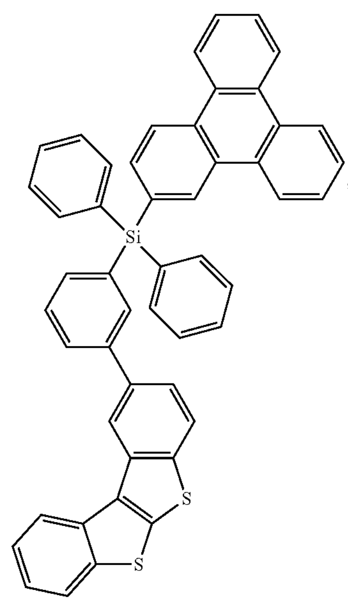
Compound 38



Compound 39



Compound 40



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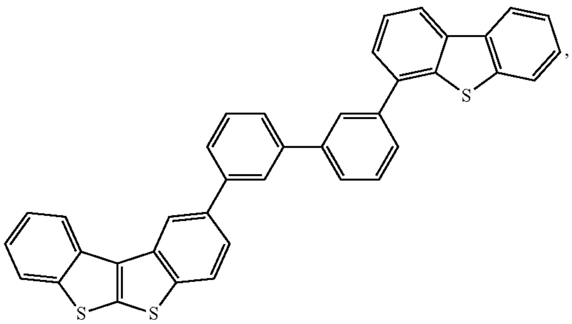
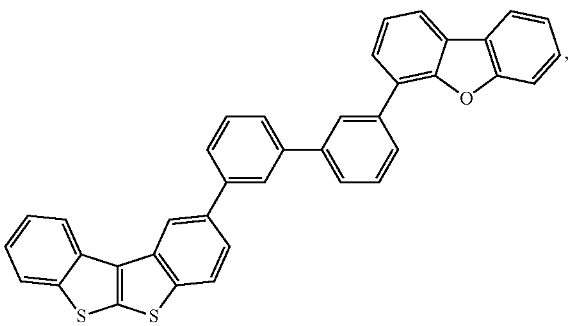
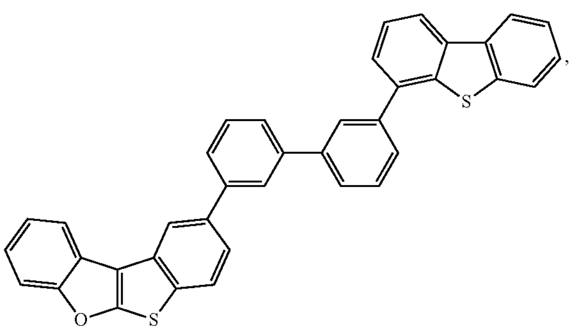
Compound 41



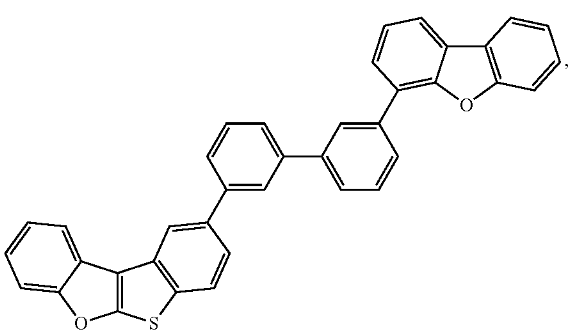
Compound 42



Compound 43



Compound 44



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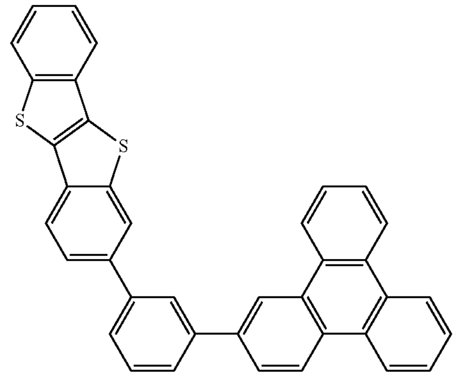
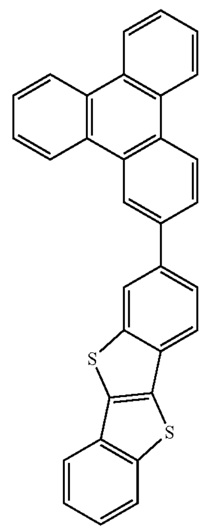
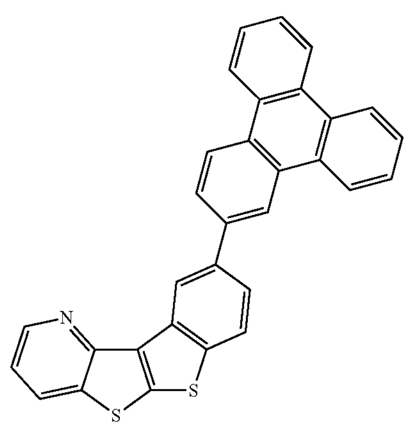
Compound 45



Compound 46



Compound 47



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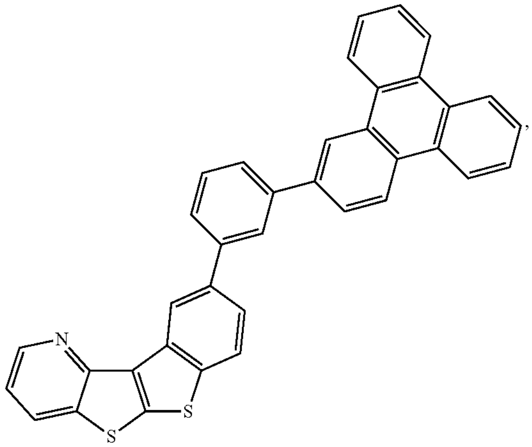
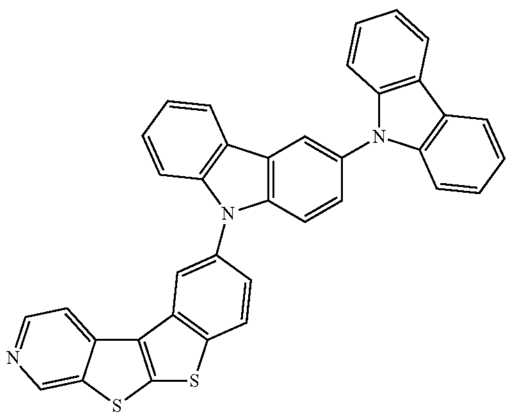
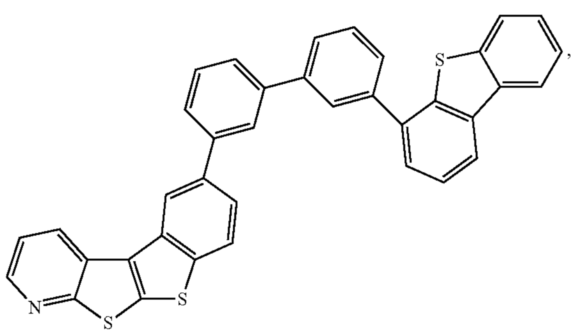
Compound 48



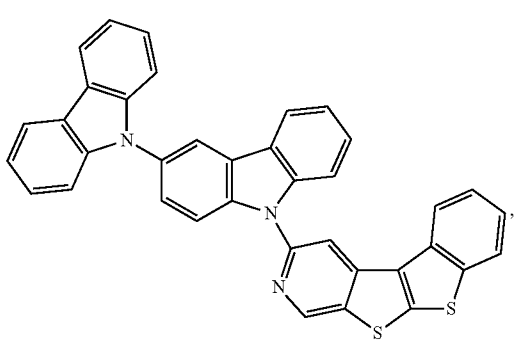
Compound 49



Compound 50



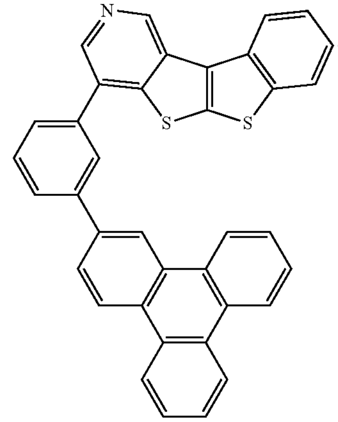
Compound 51



and

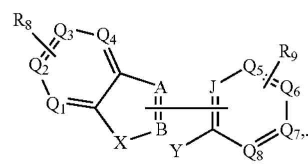
-continued

Compound 52



In one embodiment, a first device comprising an organic light emitting device, further comprising an anode, a cathode, and an organic layer, disposed between the anode and the cathode, comprising a compound having the formula:

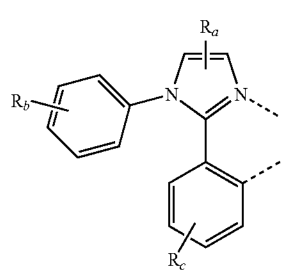
Formula I

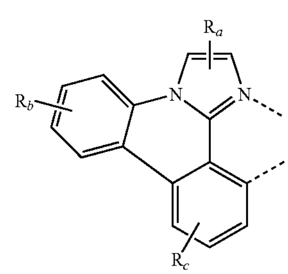


In the compound of Formula I, Q_1 to Q_8 are independently selected from CH and N, and wherein Q_1 to Q_8 may be further substituted. A is directly bonded to J and B is directly bonded to Y, or wherein A is directly bonded to Y and B is directly bonded to J. A, B, and J are carbon atoms. X and Y are independently selected from the group consisting of O, S, and Se. R_8 and R_9 independently represent mono, di, tri, tetra substitution, or no substitution. R_8 and R_9 are independently selected from the group consisting of deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof, and at least one of R_8 and R_9 is not hydrogen or deuterium.

In one embodiment, the organic layer is an emissive layer and the compound of Formula I is a host. In one embodiment, the organic layer further comprises an emissive dopant.

In one embodiment, the emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:





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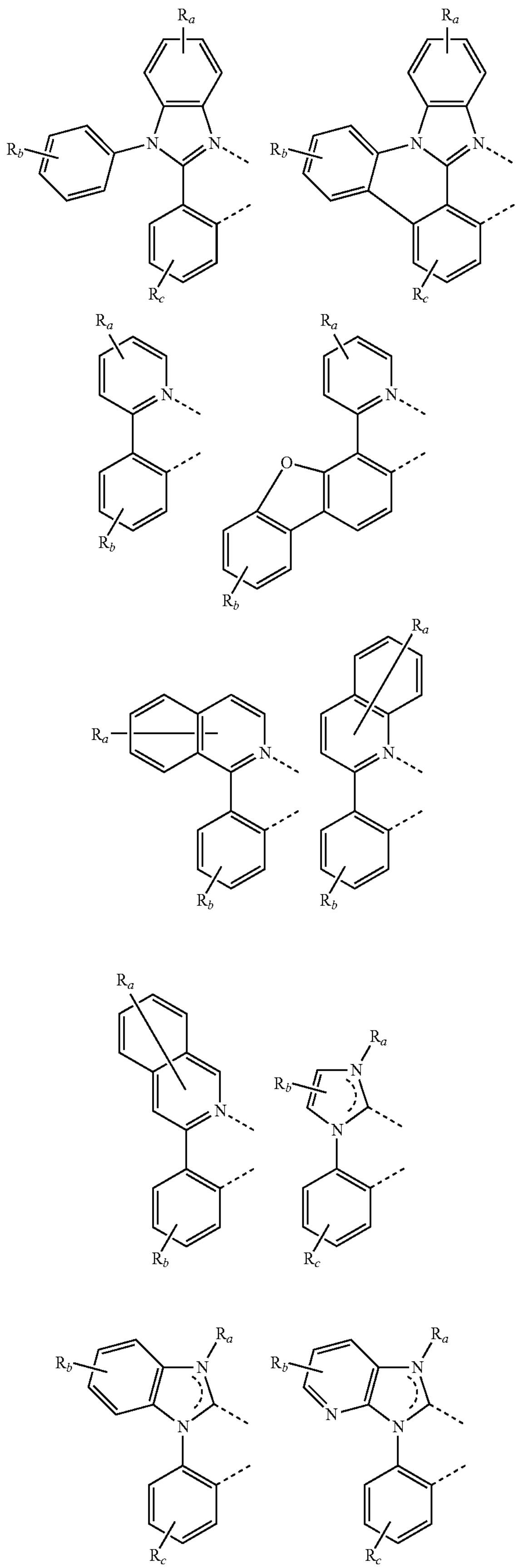

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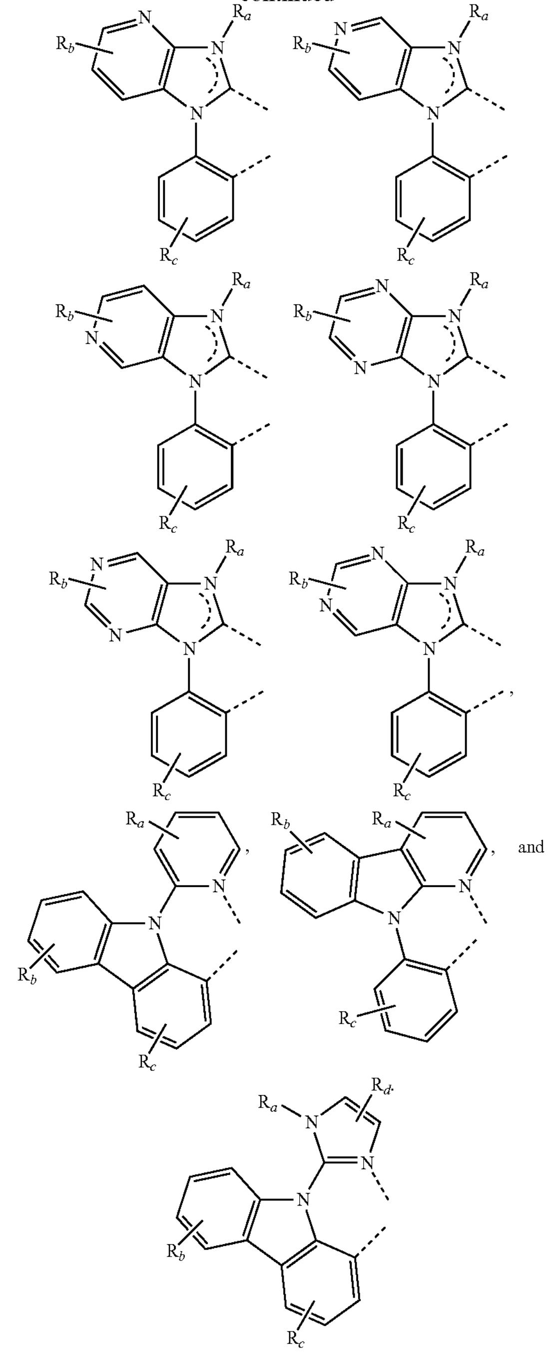


R_a, R_b, and R_c may represent mono, di, tri or tetra substitutions, or no substitution, and R_a, R_b, and R_c are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof. Two adjacent substituents of R_a, R_b, and R_c are optionally joined to form a fused ring or form a multidentate ligand.

In one embodiment, the device further comprises a second organic layer that is a non-emissive layer and the compound having Formula I is a material in the second organic layer.

In one embodiment, the second organic layer is a blocking layer and the compound having Formula I is a blocking material in the second organic layer.

In one embodiment, the first device is a consumer product. In one embodiment, the first device is an organic light-emitting device. In one embodiment, the first device comprises a lighting panel.

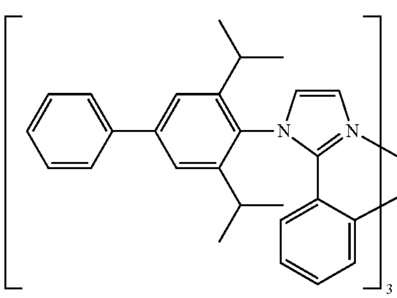
DEVICE EXAMPLES

All example devices were fabricated by high vacuum ($<10^{-7}$ Torr) thermal evaporation (VTE). The anode electrode is 800 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1,000 Å of Al. All devices are encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H_2O and O_2) immediately after fabrication, and a moisture getter was incorporated inside the package.

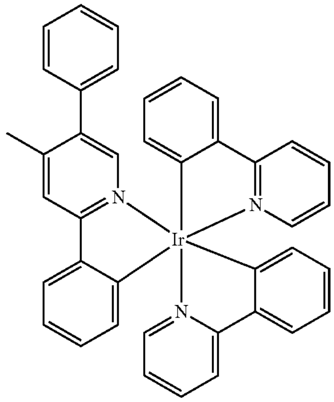
The organic stack of the device examples consisted of sequentially, from the ITO surface, 100 Å of Compound B or C as the hole injection layer (HIL), 300 Å of 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (NPD) as the hole transporting layer (HTL), 300 Å of a compound of Formula I doped in compound D as host with 12, 15, or 20 wt % of an Ir phosphorescent compound as the emissive layer (EML), 100 Å of Compound D or E as block layer (BL), 400 Å of Alq_3 (tris-8-hydroxyquinoline aluminum) as the ETL.

The device structure and data are summarized in Table 2 and Table 3 from those devices. As used herein, Compounds A, B, C, D and E have the following structures:

Compound A



Compound B



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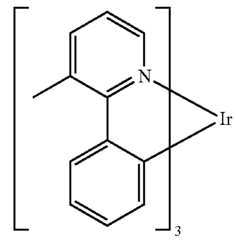
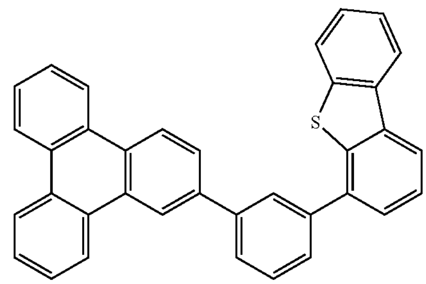
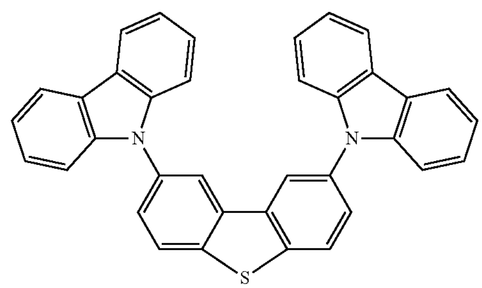
Compound C

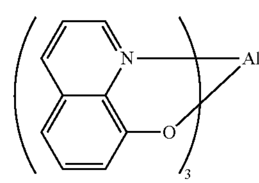


Compound D

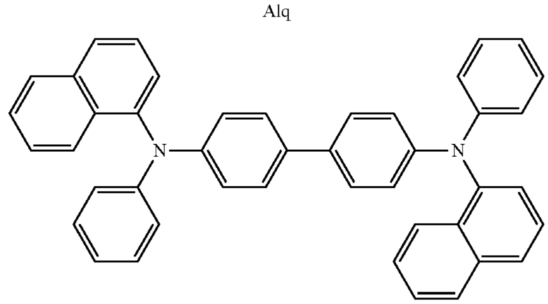


Compound E





Alq



NPD

TABLE 2

Device Structures of Devices Incorporating Compounds of Formula I						
Example	HIL	HTL	EML (300 Å, doping %)		BL	ETL
Example 1	Compound B 100 Å	NPD 300 Å	Compound 41	Compound B 12%	Compound 41 100 Å	Alq 400 Å
Example 2	Compound B 100 Å	NPD 300 Å	Compound 41	Compound B 12%	Compound D 100 Å	Alq 400 Å
Example 3	Compound B 100 Å	NPD 300 Å	Compound 41	Compound B 12%	None	Alq 450 Å
Example 4	Compound B 100 Å	NPD 300 Å	Compound 3	Compound B 12%	Compound 3 100 Å	Alq 400 Å
Example 5	Compound B 100 Å	NPD 300 Å	Compound 3	Compound B 12%	Compound D 100 Å	Alq 400 Å
Example 6	Compound B 100 Å	NPD 300 Å	Compound 3	Compound B 12%	None	Alq 450 Å
Example 7	Compound C 100 Å	NPD 300 Å	Compound 7	Compound A 15%	Compound 7 100 Å	Alq 400 Å
Example 8	Compound C 100 Å	NPD 300 Å	Compound 7	Compound A 15%	Compound E 100 Å	Alq 400 Å
Example 9	Compound C 100 Å	NPD 300 Å	Compound 7	Compound A 20%	Compound 7 100 Å	Alq 400 Å
Example 10	Compound C 100 Å	NPD 300 Å	Compound 7	Compound A 20%	Compound E 100 Å	Alq 400 Å
Comparative Example 1	Compound B 100 Å	NPD 300 Å	Compound D	Compound B 12%	Compound D 100 Å	Alq 400 Å
Comparative Example 2	Compound B 100 Å	NPD 300 Å	Compound D	Compound B 12%	None	Alq 450 Å

TABLE 3

VTE Device Data for Compounds of Formula I								
	x	y	λ_{max} (nm)	FWHM (nm)	Voltage (V)	LE (Cd/A)	EQE (%)	PE (lm/W)
Example 1	0.319	0.628	522	64	6.4	45.5	12.6	22.1
Example 2	0.321	0.628	522	66	5.8	62.9	17.4	33.8
Example 3	0.318	0.628	522	64	7.5	15.2	4.2	6.4
Example 4	0.348	0.612	528	74	6.4	43.5	12	21.5
Example 5	0.365	0.602	532	78	6.9	33.9	9.4	15.3
Example 6	0.359	0.605	528	76	8	19	5.3	7.5
Example 7	0.187	0.421	476	60	9.4	26.8	11.2	9.0
Example 8	0.185	0.414	474	60	7.9	31.8	13.4	12.6
Example 9	0.184	0.415	476	60	8.2	28.6	12.1	10.9
Example 10	0.180	0.406	474	58	6.9	39.2	16.9	17.7
Comparative Example 1	0.324	0.626	522	66	6.8	62.2	17.2	28.9
Comparative Example 2	0.323	0.626	522	66	7.6	24.7	6.8	10.2

Table 3 is a summary of the device data. The luminous efficiency (LE), external quantum efficiency (EQE) and power efficiency (PE) were measured at 1000 nits. Advantageously, the data indicates that the hosts containing benzo[b]benzo[4,5]thieno[3,2,d]thiophene core can be used as either green emitter hosts (Compound 3 and 41) or as blue emitter hosts (Compound 7). Thus, compounds of Formula I are efficient hosts when used in devices intended to emit blue or green light. Additionally, no energy quenching was observed with the novel hosts in the blue device as expected.

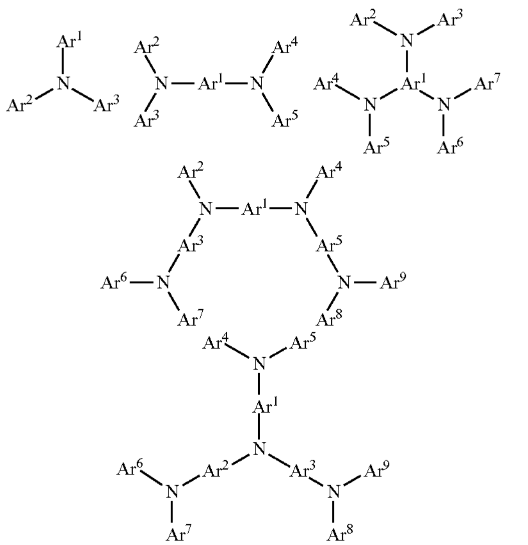
Combination with Other Materials

The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

HIL/HTL:

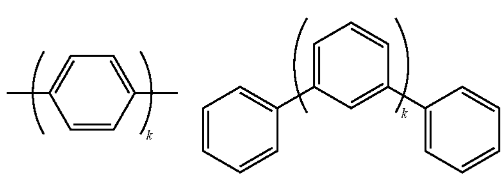
A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphryin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and sliane derivatives; a metal oxide derivative, such as MoO_x; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:



Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

In one aspect, Ar^1 to Ar^9 is independently selected from the group consisting of:



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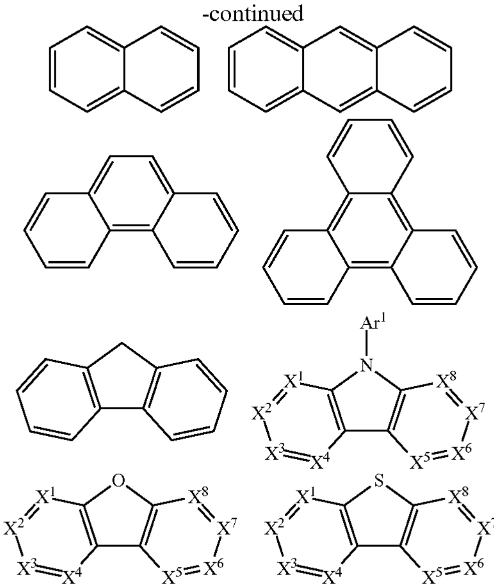
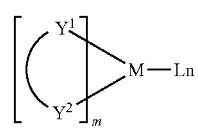


k is an integer from 1 to 20; X^1 to X^8 is C (including CH) or N; Ar^1 has the same group defined above.

Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:



M is a metal, having an atomic weight greater than 40; $(Y^1\text{-}Y^2)$ is a bidentate ligand, Y^1 and Y^2 are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

In one aspect, $(Y^1\text{-}Y^2)$ is a 2-phenylpyridine derivative.

In another aspect, $(Y^1\text{-}Y^2)$ is a carbene ligand.

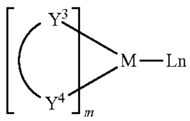
In another aspect, M is selected from Ir, Pt, Os, and Zn.

In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc^+/Fc couple less than about 0.6 V.

Host:

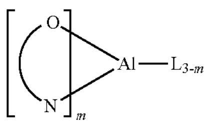
The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. While the Table below categorizes host materials as preferred for devices that emit various colors, any host material may be used with any dopant so long as the triplet criteria is satisfied.

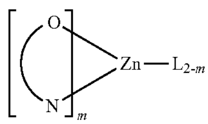
Examples of metal complexes used as host are preferred to have the following general formula:



M is a metal; (Y^3-Y^4) is a bidentate ligand, Y^3 and Y^4 are independently selected from C, N, O, P, and S; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and m+n is the maximum number of ligands that may be attached to the metal.

In one aspect, the metal complexes are:





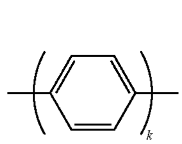
(O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

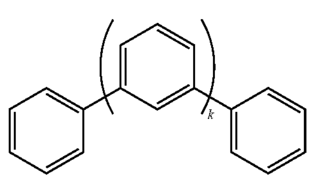
In another aspect, M is selected from Ir and Pt.

In a further aspect, (Y^3-Y^4) is a carbene ligand.

Examples of organic compounds used as host are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atome, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

In one aspect, host compound contains at least one of the following groups in the molecule:





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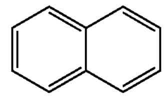

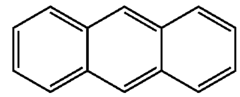

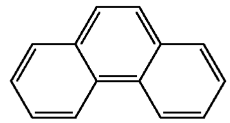

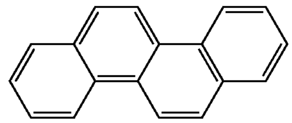

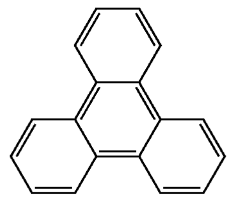

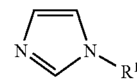

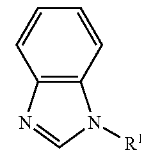

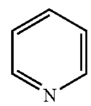

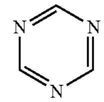

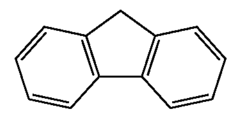

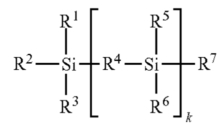

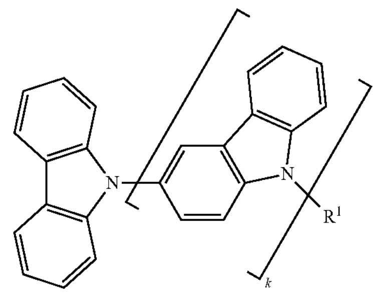

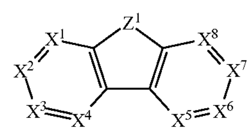

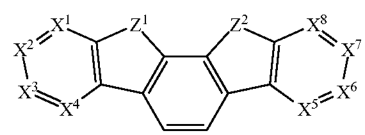

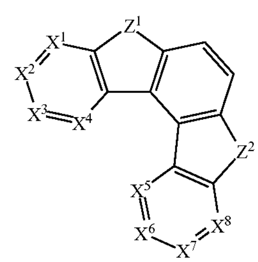

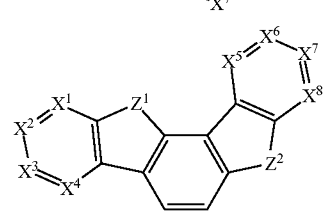

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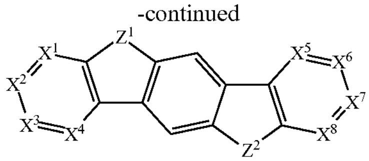
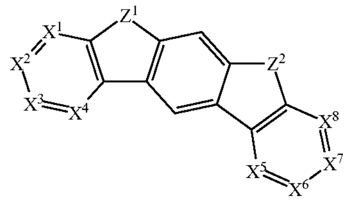




R^1 to R^7 is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

k is an integer from 0 to 20.

X^1 to X^8 is selected from C (including CH) or N.

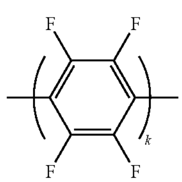
Z^1 and Z^2 is selected from NR^1, O, or S.

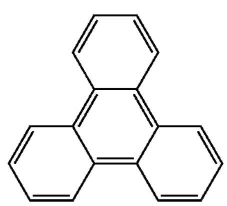
HBL:

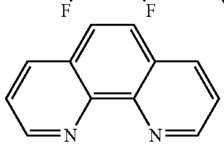
A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED.

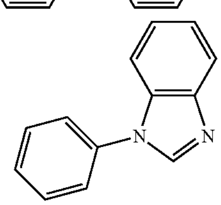
In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

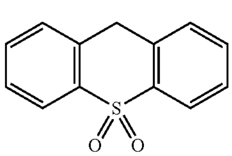
In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

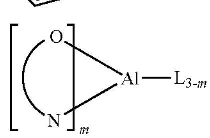










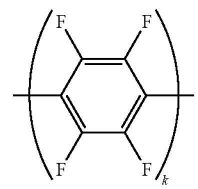


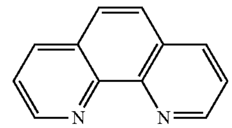
k is an integer from 0 to 20; L is an ancillary ligand, m is an integer from 1 to 3.

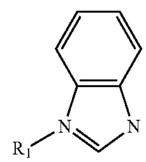
ETL:

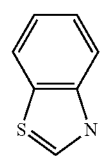
Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

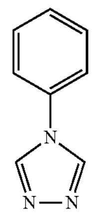
In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

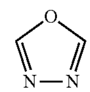


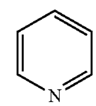


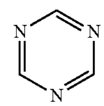


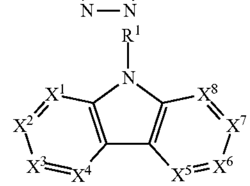


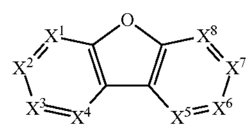


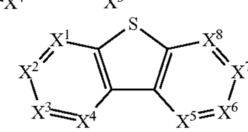


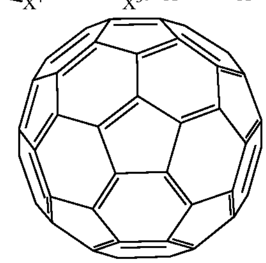


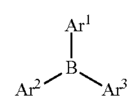












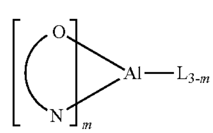
R^1 is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

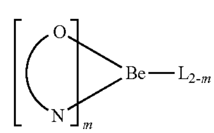
Ar^1 to Ar^3 has the similar definition as Ar's mentioned above.

k is an integer from 0 to 20.

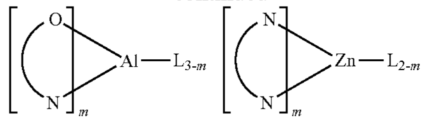
X^1 to X^8 is selected from C (including CH) or N.

In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:





-continued



(O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L is an ancillary ligand; m is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated.

In addition to and/or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exiton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed in Table 2 below. Table 2 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

TABLE 2

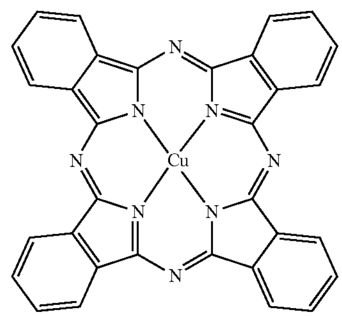
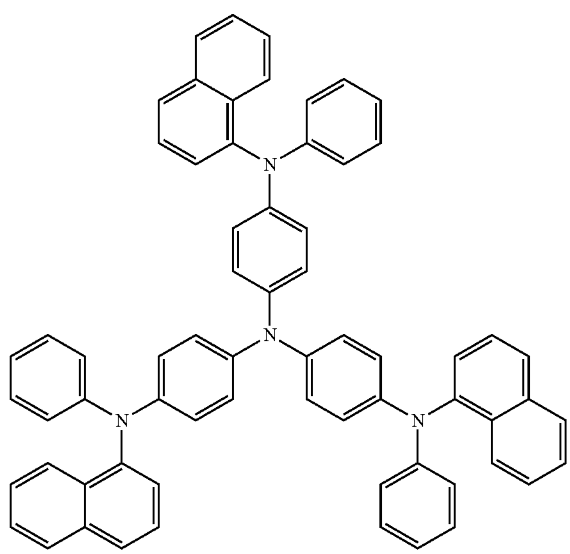
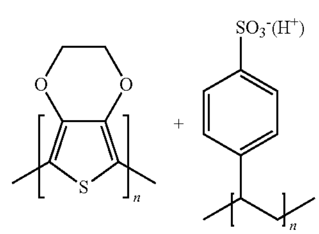
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
CF_x Fluorohydrocarbon polymer	$-\!\left[CH_xF_y\right]_n\!-$	Appl. Phys. Lett. 78, 673 (2001)
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polypthiophene)		Synth. Met. 87, 171 (1997) WO2007002683

TABLE 2-continued

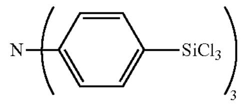
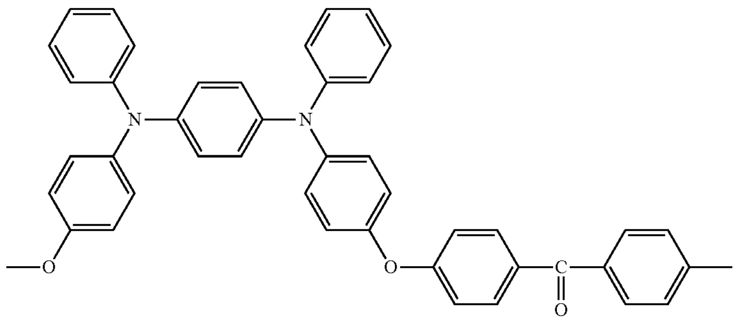
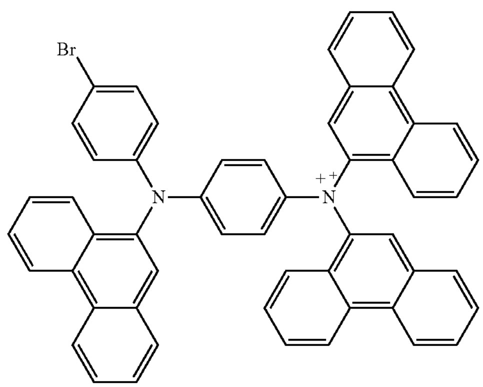
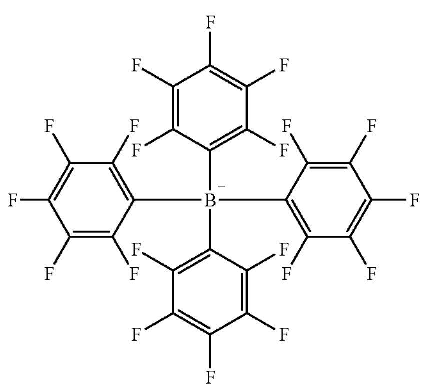
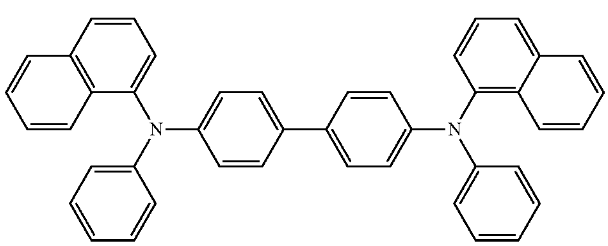
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phosphonic acid and sliane SAMs		US20030162053
Triarylamine or polythiophene polymers with conductivity dopants	 and  	EP1725079A1
Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides	 + MoO_x	US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009

TABLE 2-continued

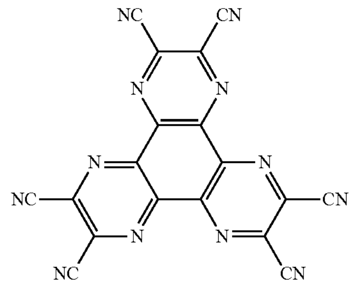
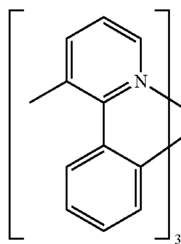
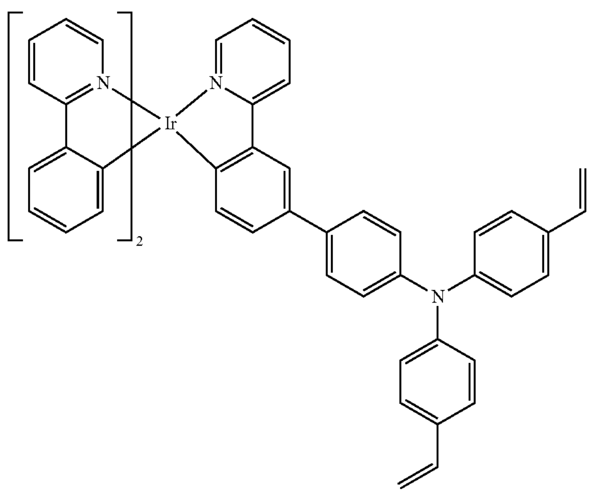
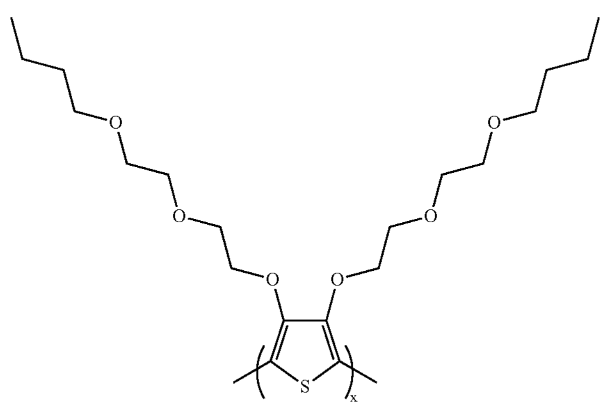
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
n-type semiconducting organic complexes		US20020158242
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Polythiophene based polymers and copolymers		WO 2011075644 EP2350216

TABLE 2-continued

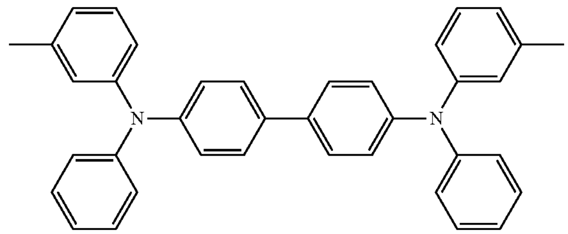
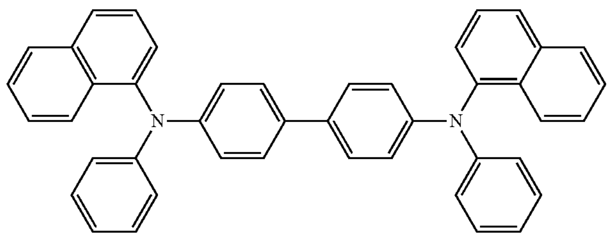
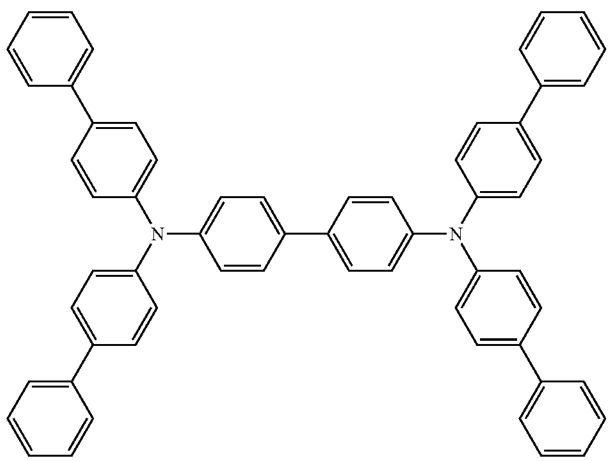
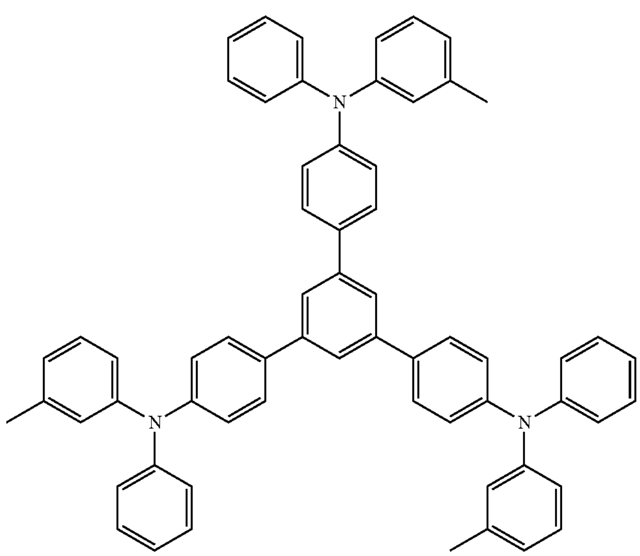
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole transporting materials	
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987)
		U.S. Pat. No. 5,061,569
		EP650955
		J. Mater. Chem. 3, 319 (1993)

TABLE 2-continued

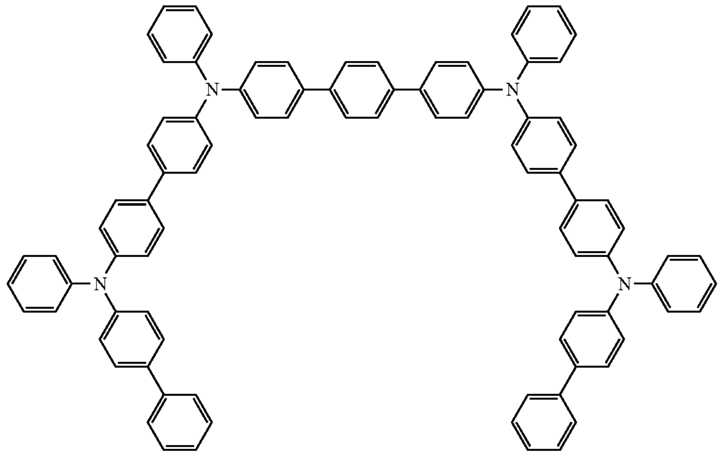
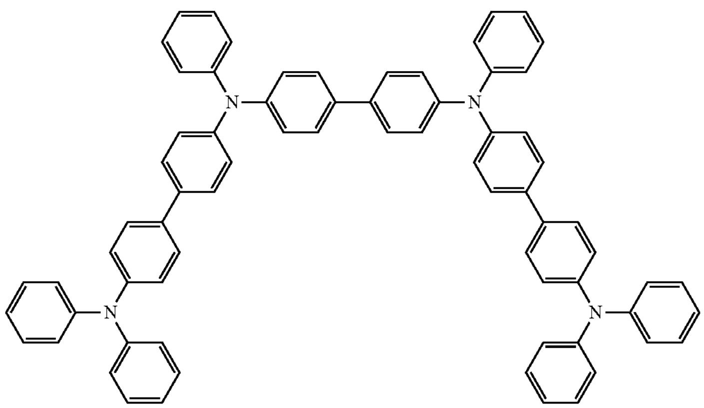
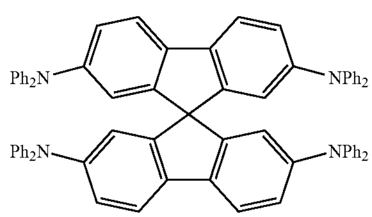
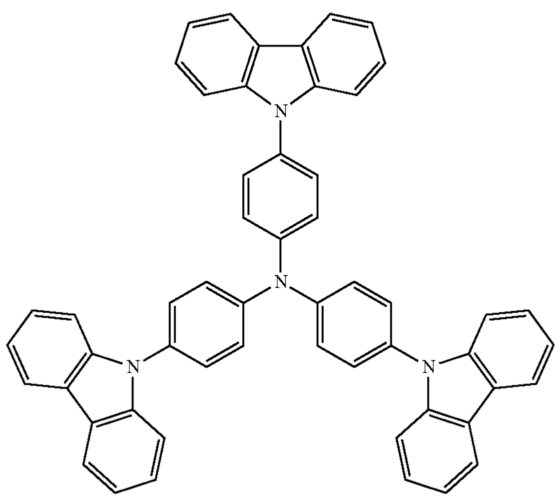
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
		Appl. Phys. Lett. 90, 183503 (2007)
Triaylamine on spirofluorene core		Synth. Met. 91, 209 (1997)
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572

TABLE 2-continued

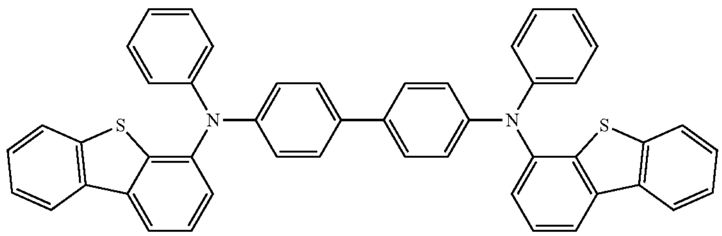
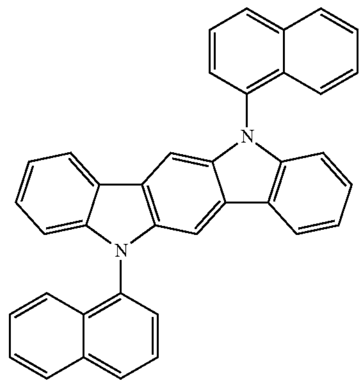
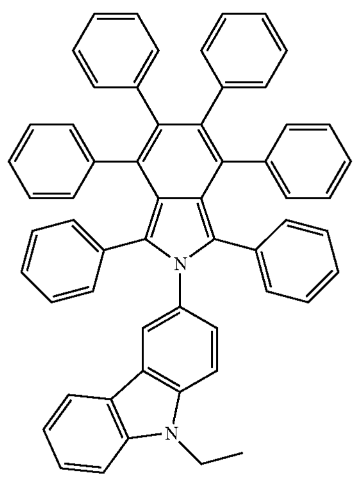
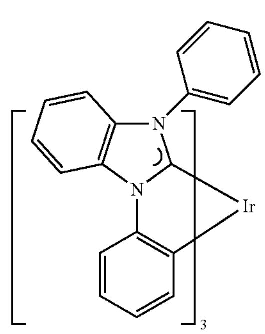
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triarylamine with (di)benzothiophene/ (di)benzofuran		US20070278938, US20080106190 US20110163302
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)
Metal carbene complexes		US20080018221

TABLE 2-continued

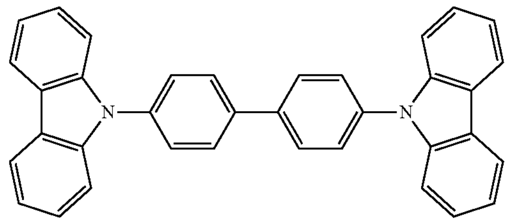
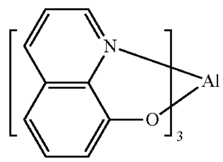
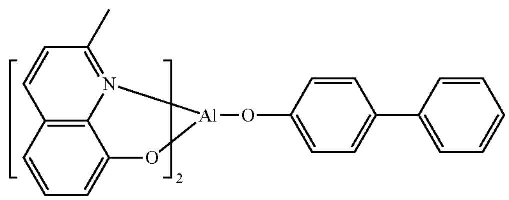
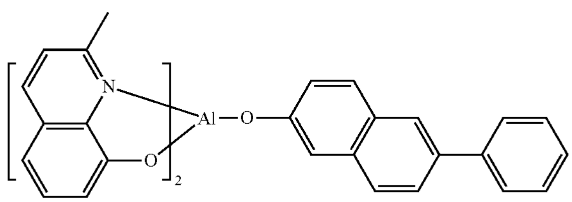
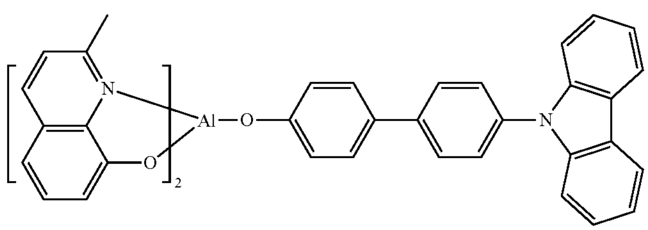
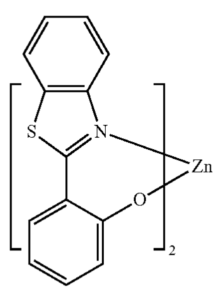
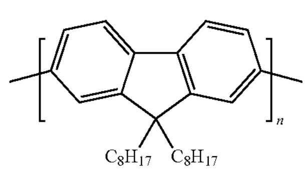
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Phosphorescent OLED host materials Red hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxyquinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194
		WO2005014551
		WO2006072002
Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)

TABLE 2-continued

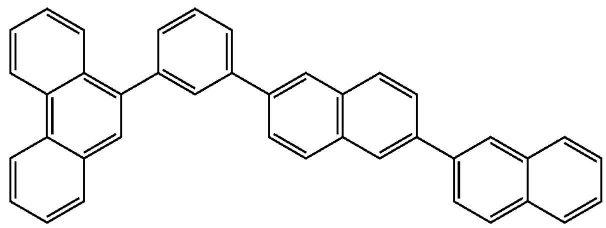
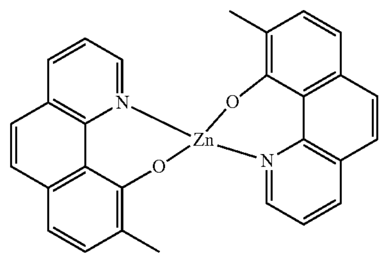
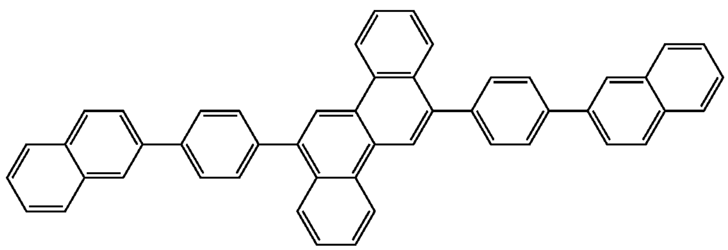
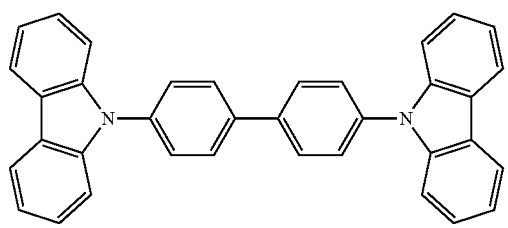
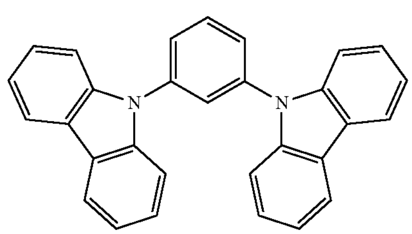
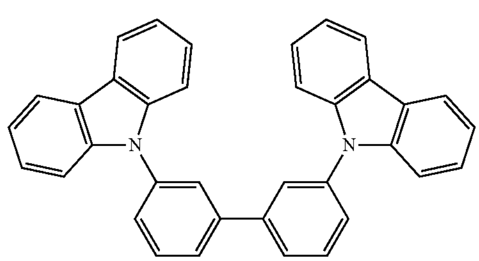
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
Zinc complexes		WO2010056066
Crysene based compounds		WO2011086863
	Green hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
		US20030175553
		WO2001039234

TABLE 2-continued

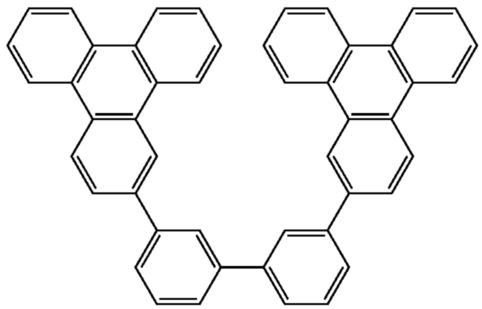
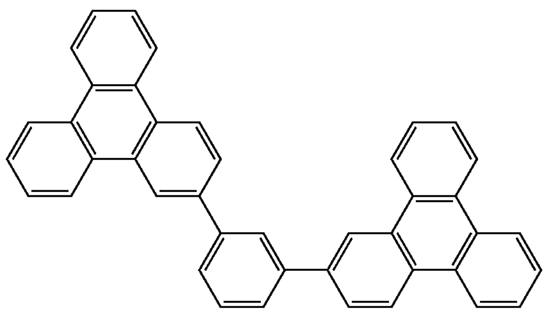
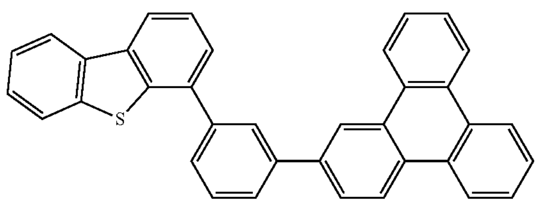
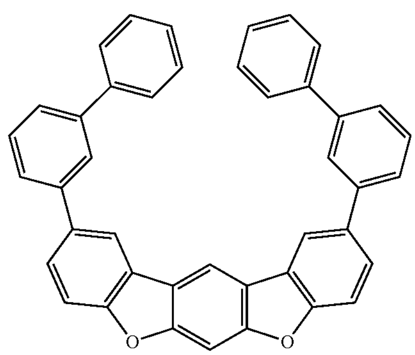
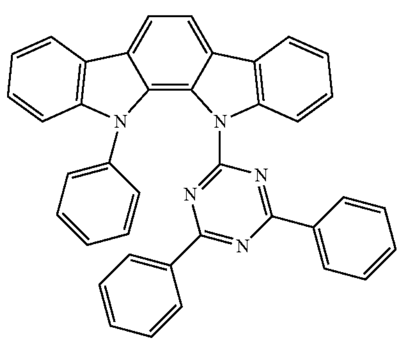
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aryltriphenylene compounds		US20060280965
		US20060280965
		WO2009021126
Poly-fused heteroaryl compounds		US20090309488 US20090302743 US20100012931
Donor acceptor type molecules		WO2008056746

TABLE 2-continued

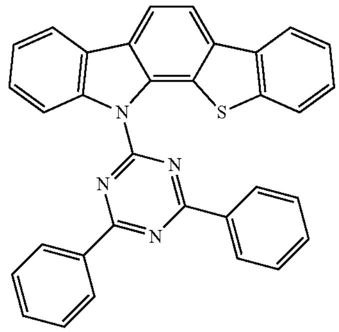
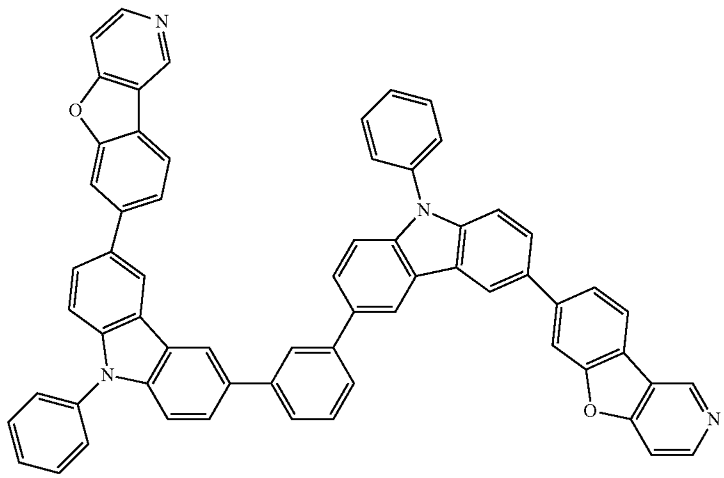
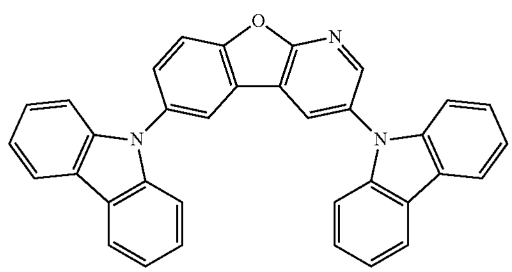
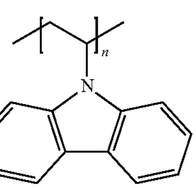
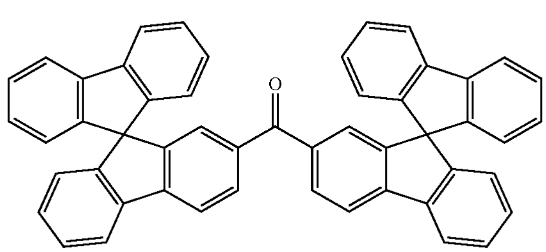
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2010107244
Aza-carbazole/ DBT/DBF		JP2008074939
		US20100187984
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
Spirofluorene compounds		WO2004093207

TABLE 2-continued

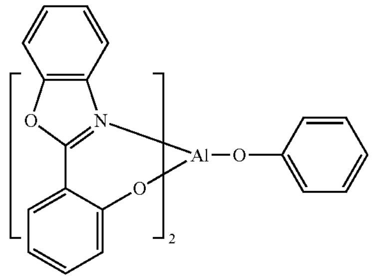
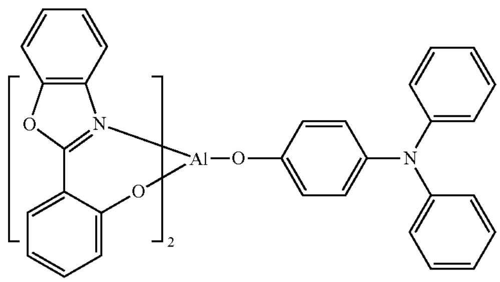
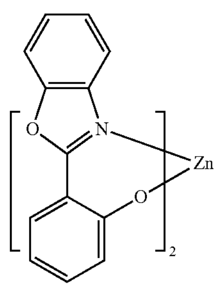
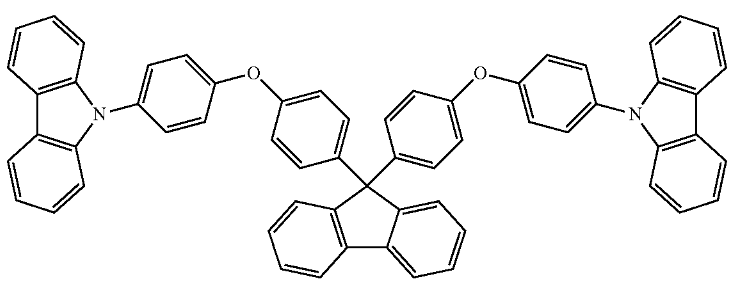
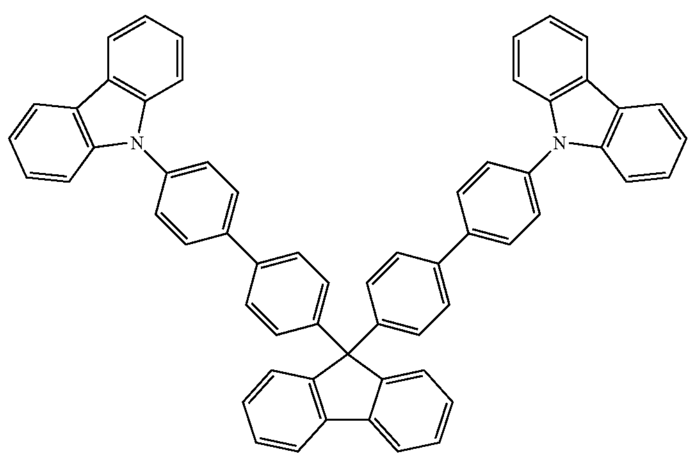
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal phenoxybenzooxazole compounds		WO2005089025
		WO2006132173
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297

TABLE 2-continued

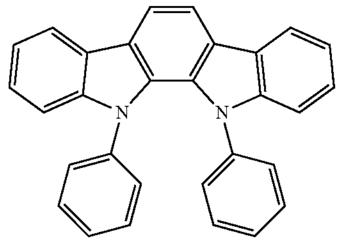
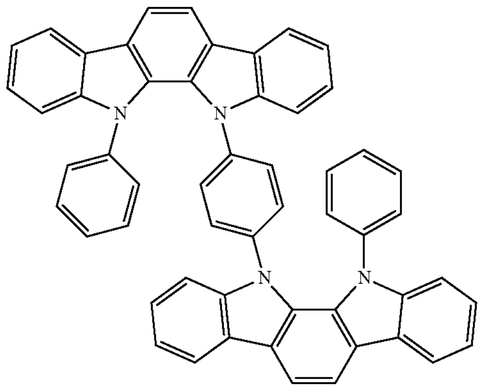
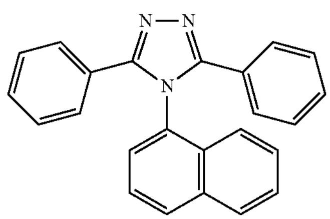
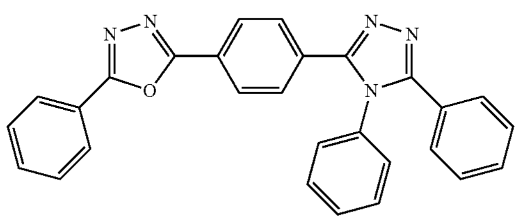
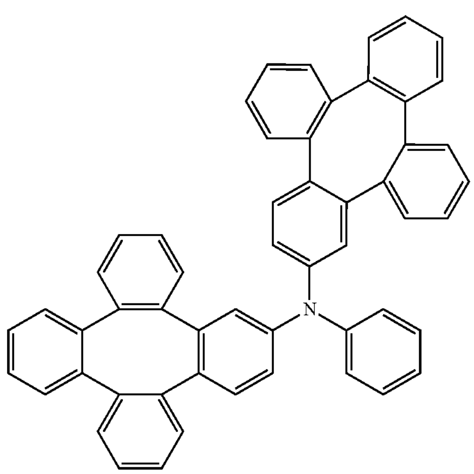
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocabazoles		WO2007063796
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
		WO2004107822
Tetraphenylene complexes		US20050112407

TABLE 2-continued

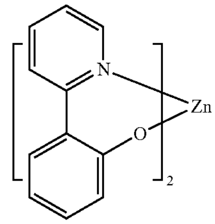
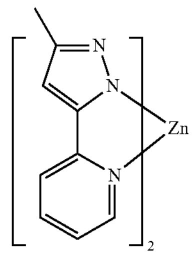
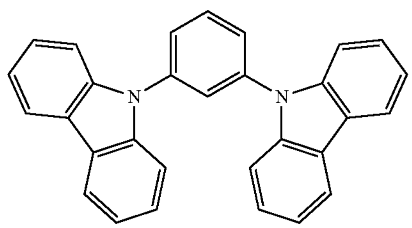
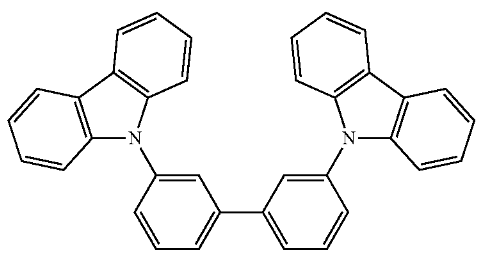
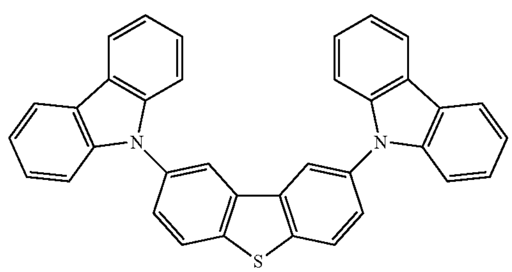
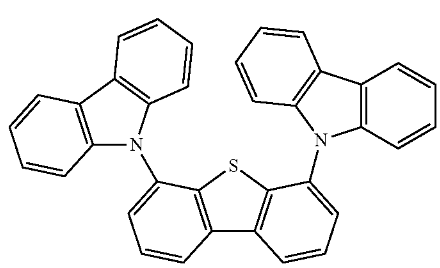
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal phenoxypyridine compounds		WO2005030900
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267
	Blue hosts	
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359
Dibenzothiophene/ Dibenzofuran-carbazole compounds		WO2006114966, US20090167162
		US20090167162

TABLE 2-continued

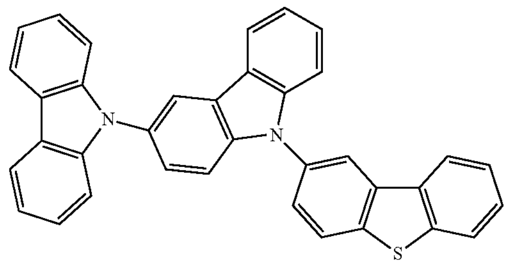
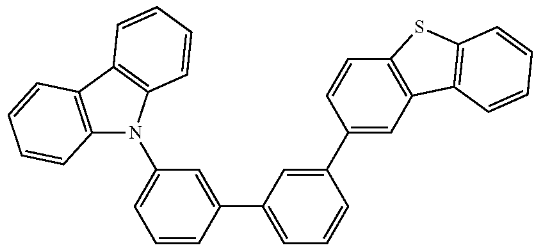
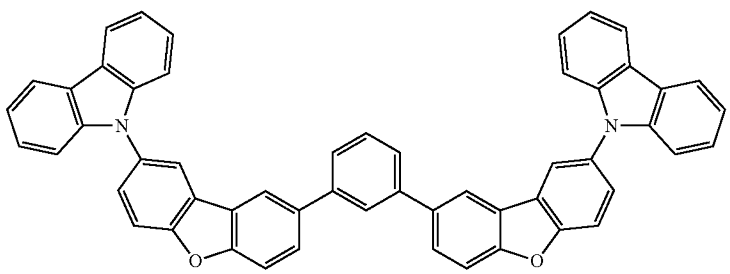
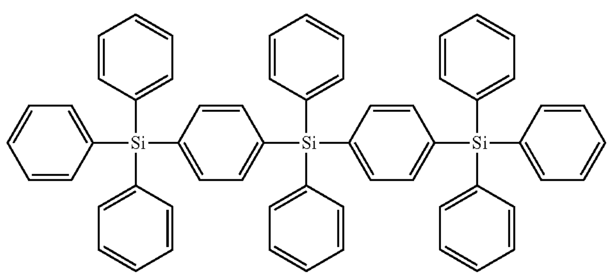
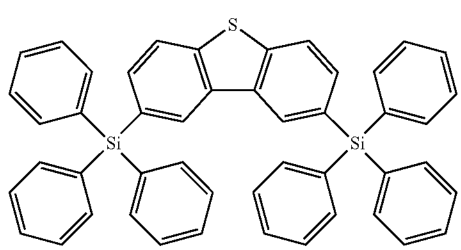
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2009086028
		US20090030202, US20090017330
		US20100084966
Silicon aryl compounds		US20050238919
		WO2009003898

TABLE 2-continued

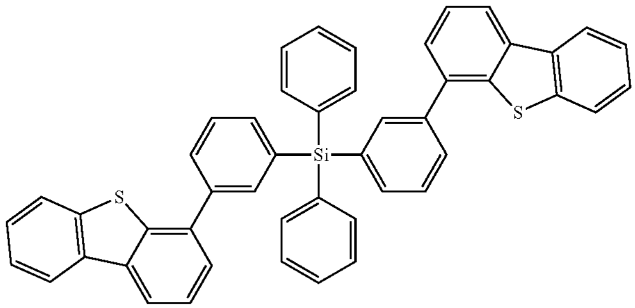
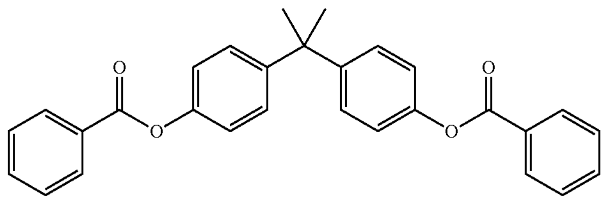
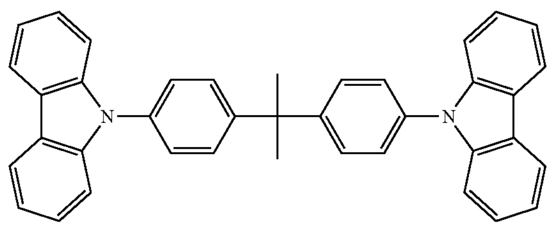
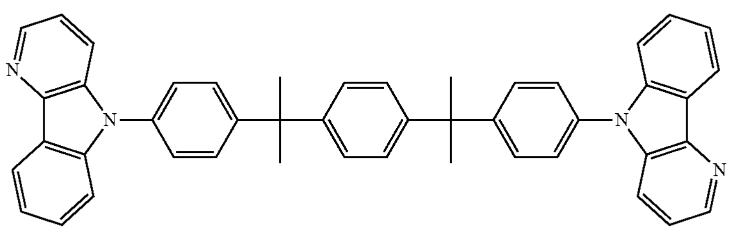
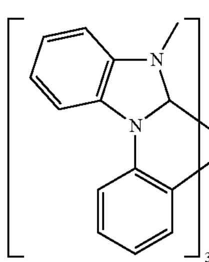
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon/Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
Carbazole linked by non-conjugated groups		US20040115476
Aza-carbazoles		US20060121308
High triplet metal organometallic complex		U.S. Pat. No. 7,154,114

TABLE 2-continued

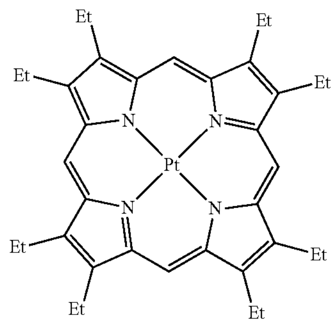
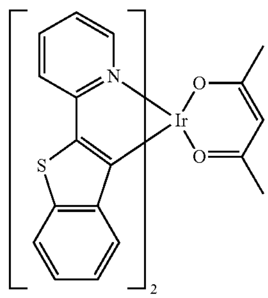
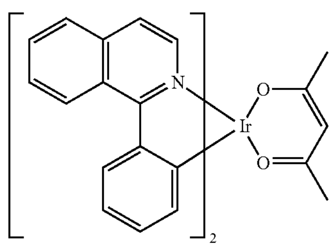
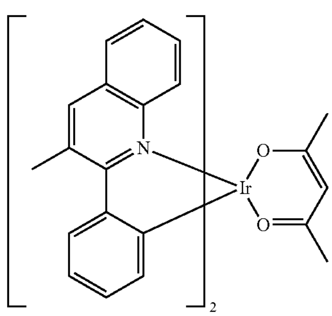
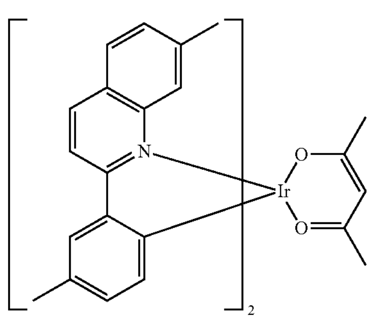
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Phosphorescent dopants Red dopants	
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
		US2006835469
		US2006835469
		US20060202194

TABLE 2-continued

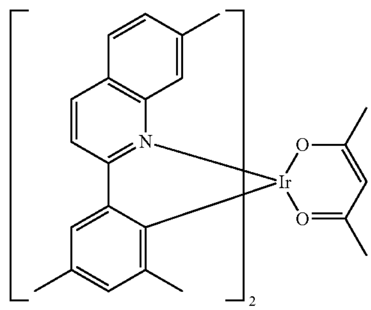
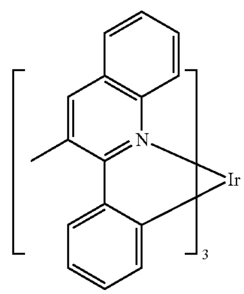
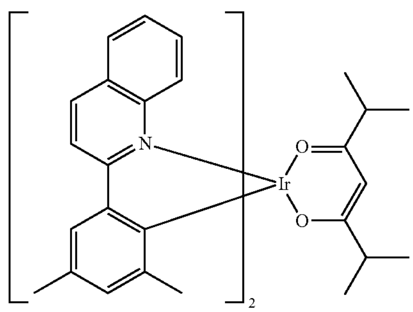
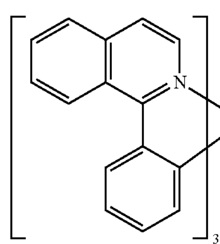
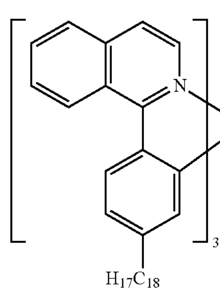
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060202194
		US20070087321
		US20080261076 US20100090591
		US20070087321
		Adv. Mater. 19, 739 (2007)

TABLE 2-continued

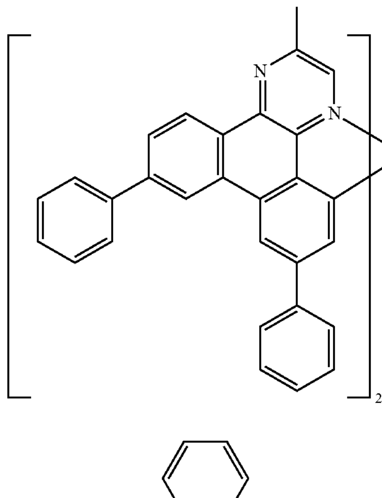
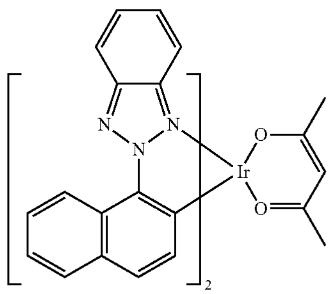
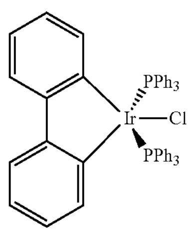
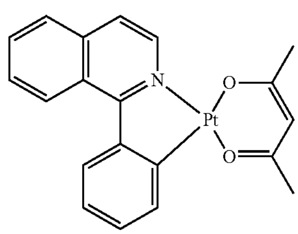
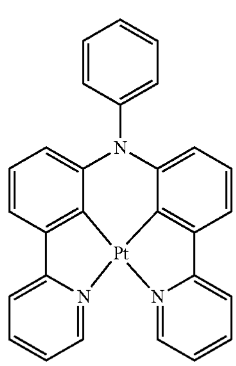
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2009100991
		WO2008101842
		U.S. Pat. No. 7,232,618
Platinum(II) organometallic complexes		WO2003040257
		US20070103060

TABLE 2-continued

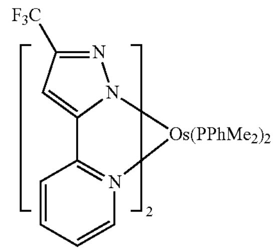
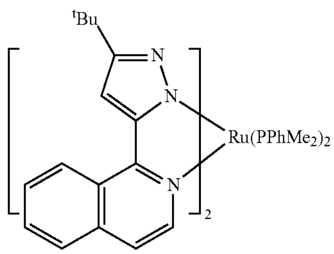
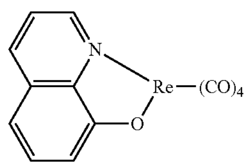
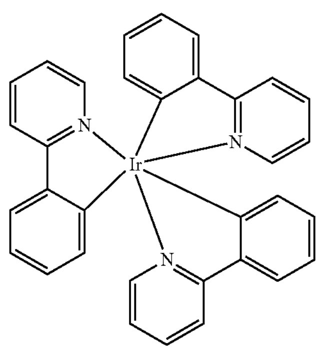
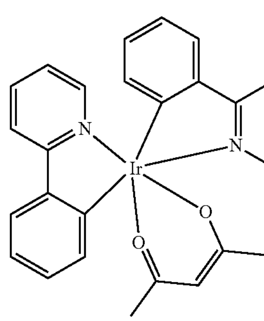
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osminum(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673
	Green dopants	
Iridium(III) organometallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656

TABLE 2-continued

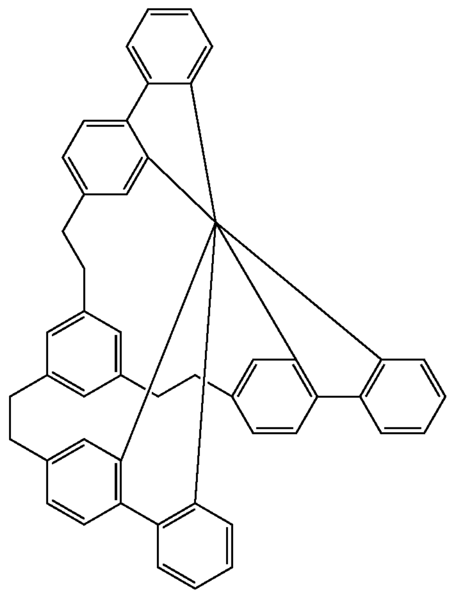
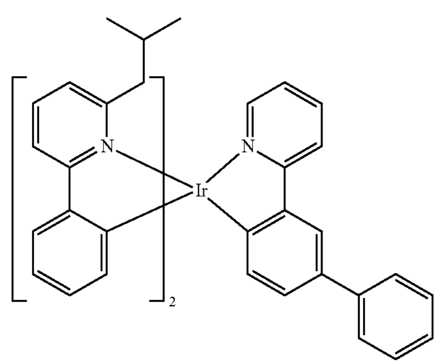
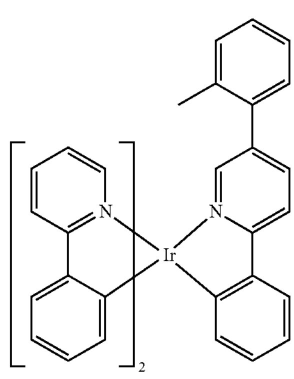
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7,332,232
		US20090108737
		WO2010028151

TABLE 2-continued

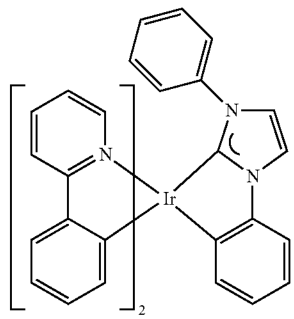
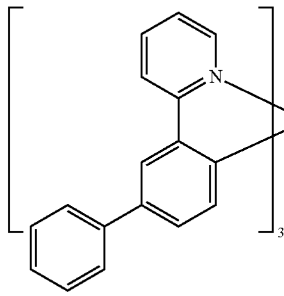
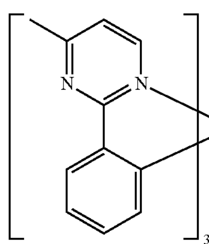
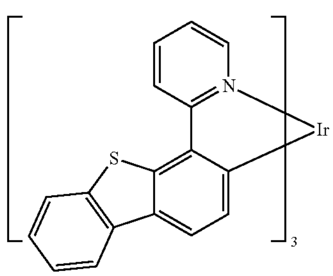
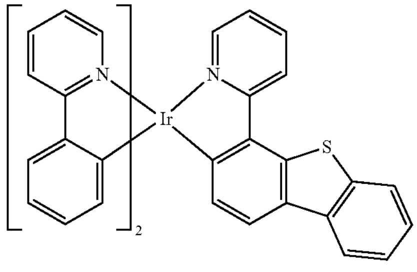
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		EP1841834B
		US20060127696
		US20090039776
		U.S. Pat. No. 6,921,915
		US20100244004

TABLE 2-continued

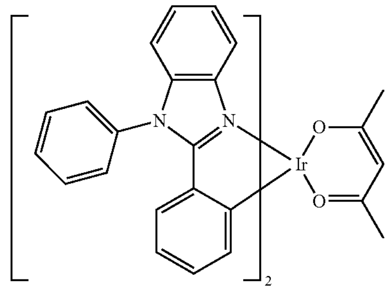
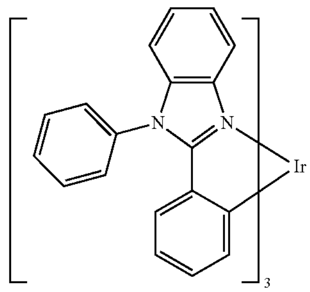
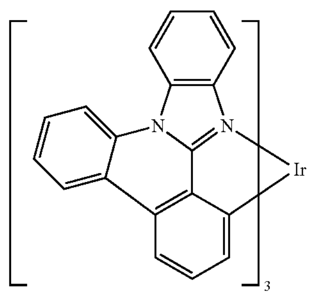
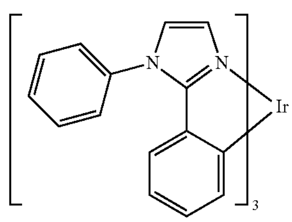
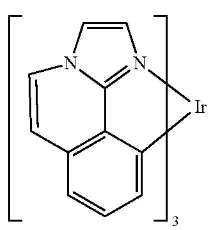
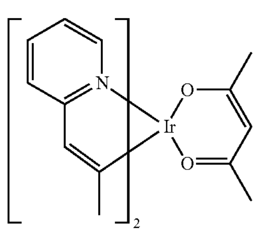
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 6,687,266
		Chem. Mater. 16, 2480 (2004)
		US20070190359
		US 20060008670 JP2007123392
		WO2010086089, WO2011044988
		Adv. Mater. 16, 2003 (2004)

TABLE 2-continued

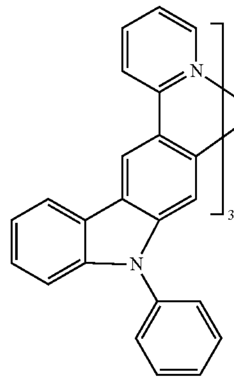
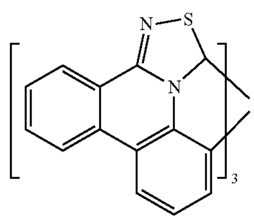
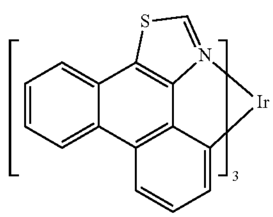
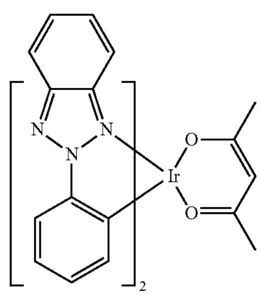
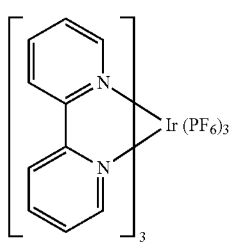
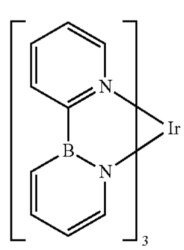
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 2006, 45, 7800
		WO2009050290
		US20090165846
		US20080015355
		US20010015432
		US20100295032

TABLE 2-continued

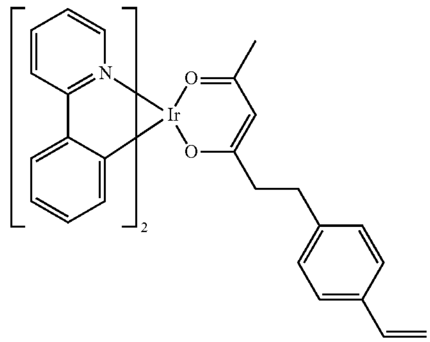
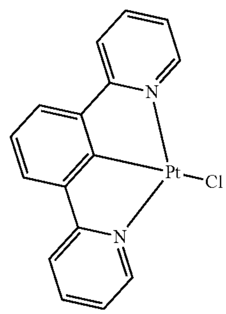
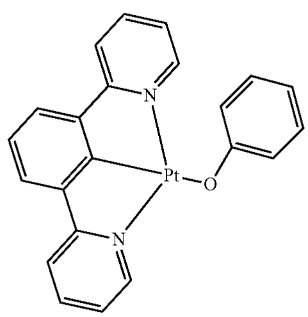
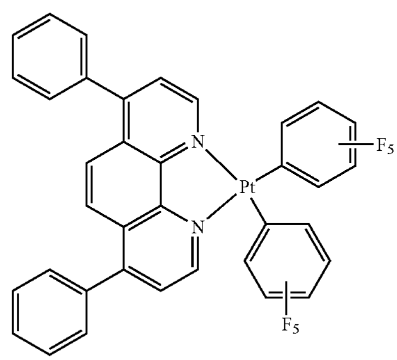
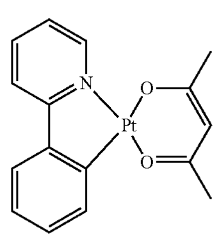
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Monomer for polymeric metal organometallic compounds		U.S. Pat. No. 7,250,226, U.S. Pat. No. 7,396,598
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645

TABLE 2-continued

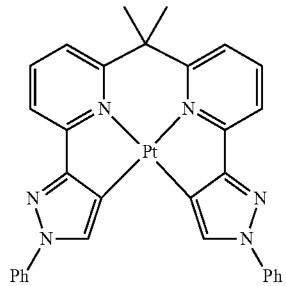
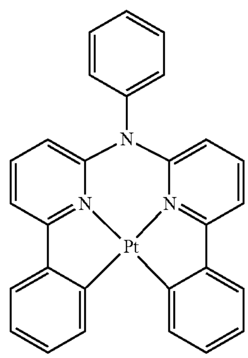
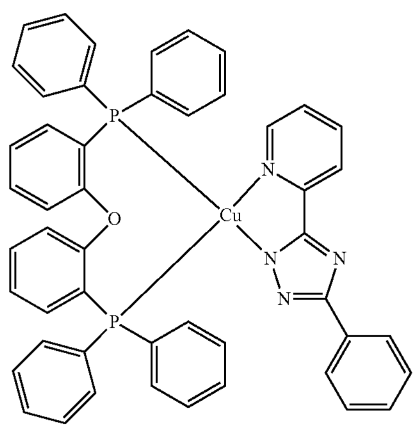
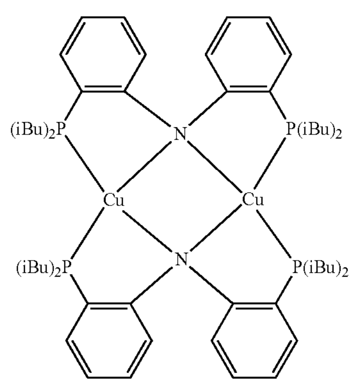
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060263635
		US20060182992 US20070103060
Cu complexes		WO2009000673
		US20070111026

TABLE 2-continued

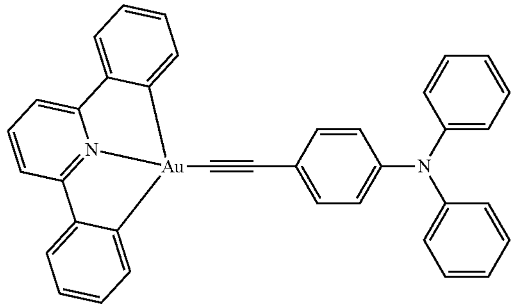
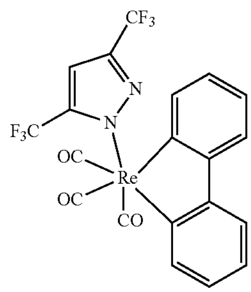
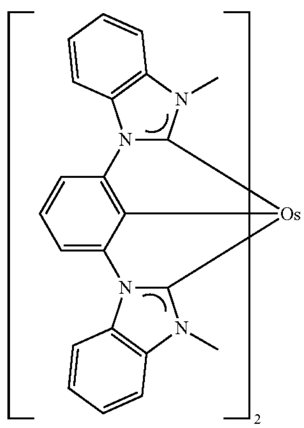
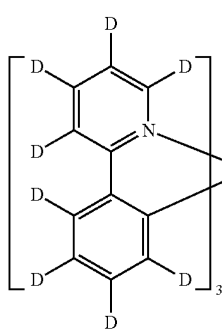
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)
Osmium(II) complexes		U.S. Pat. No. 7,279,704
Deuterated organometallic complexes		US20030138657

TABLE 2-continued

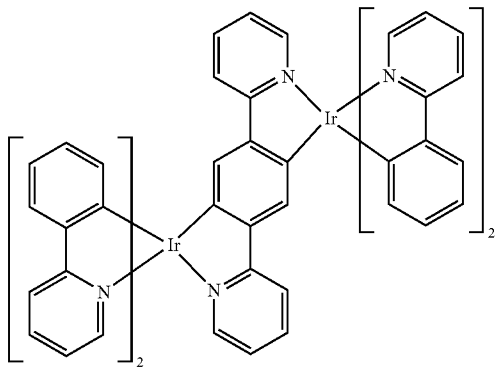
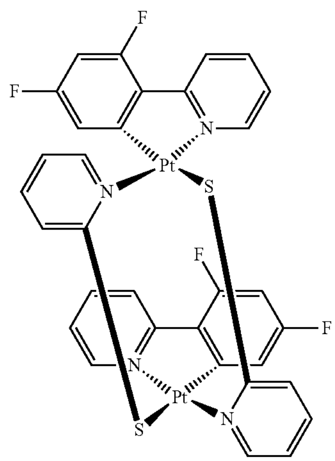
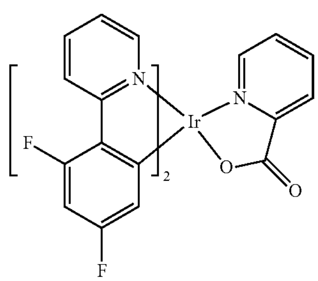
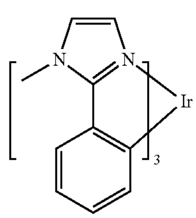
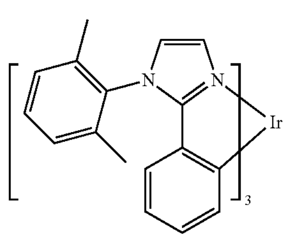
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Organometallic complexes with two or more metal centers		US20030152802
		U.S. Pat. No. 7,090,928
	Blue dopants	
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333

TABLE 2-continued

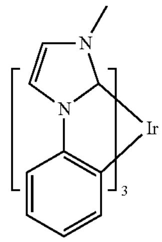
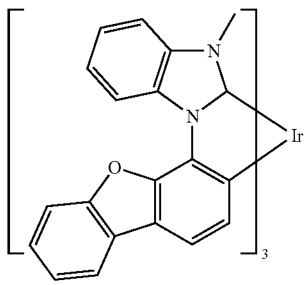
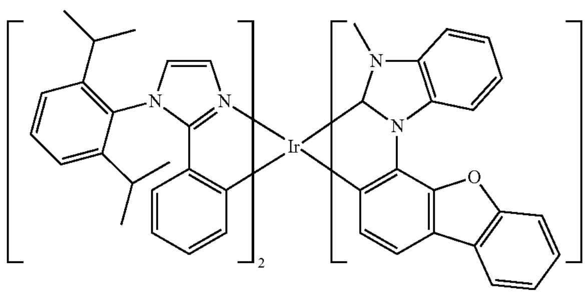
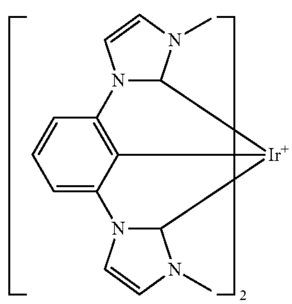
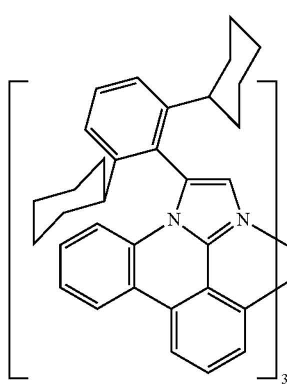
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7,393,599, WO2006056418, US20050260441, WO2005019373
		U.S. Pat. No. 7,534,505
		WO2011051404
		U.S. Pat. No. 7,445,855
		US20070190359, US20080297033 US20100148663

TABLE 2-continued

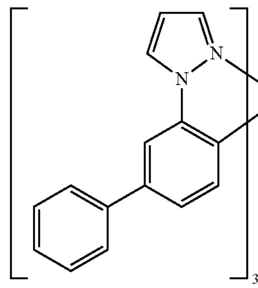
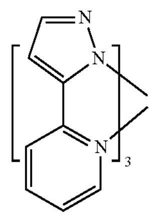
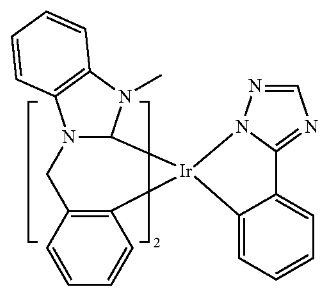
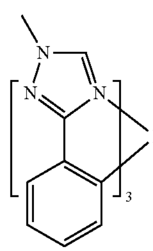
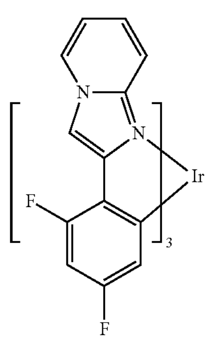
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		U.S. Pat. No. 7,338,722
		US20020134984
		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)

TABLE 2-continued

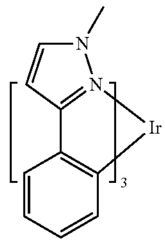
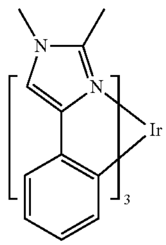
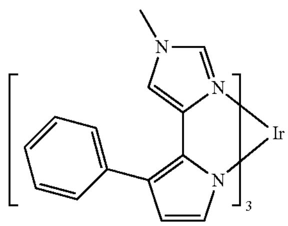
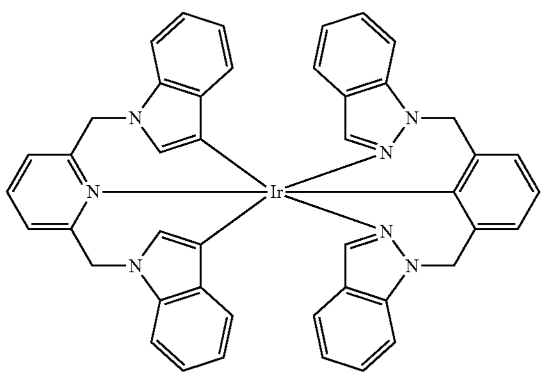
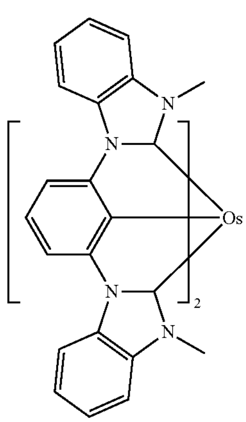
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2005123873
		WO2005123873
		WO2007004380
		WO2006082742
Osmium(II) complexes		U.S. Pat. No. 7,279,704

TABLE 2-continued

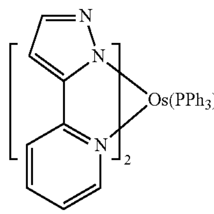
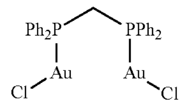
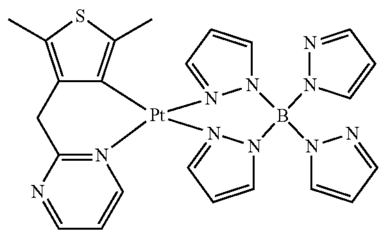
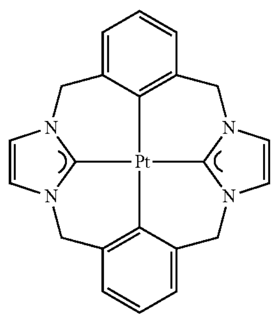
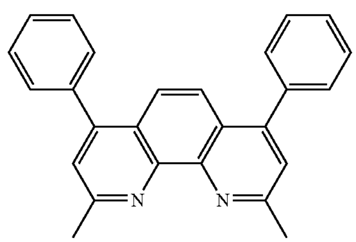
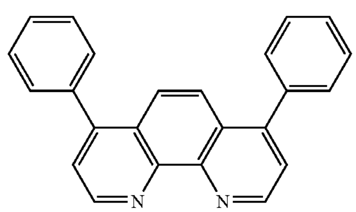
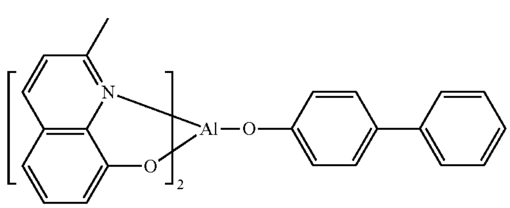
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Organometallics 23, 3745 (2004)
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum(II) complexes		WO2006098120, WO2006103874
Pt tetradentate complexes with at least one metal-carbene bond		U.S. Pat. No. 7,655,323
	Exciton/hole blocking layer materials	
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)

TABLE 2-continued

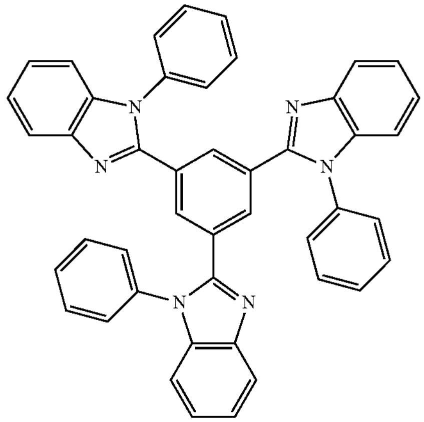
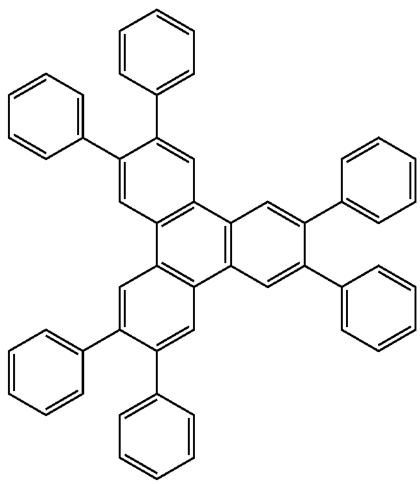
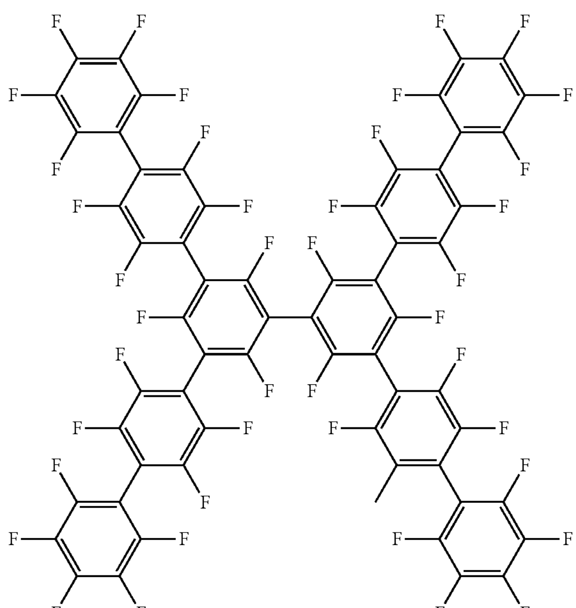
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
Triphenylene compounds		US20050025993
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)

TABLE 2-continued

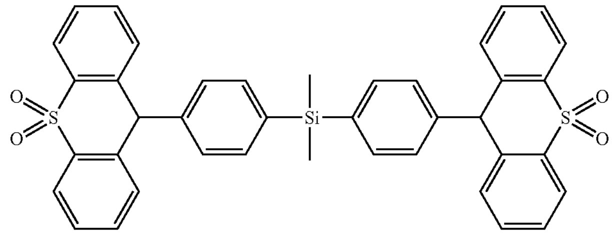
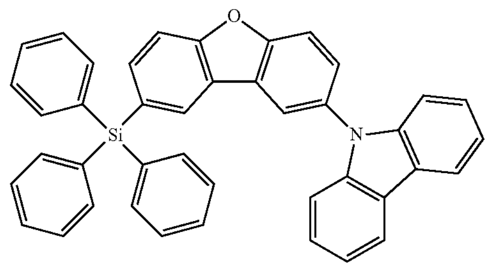
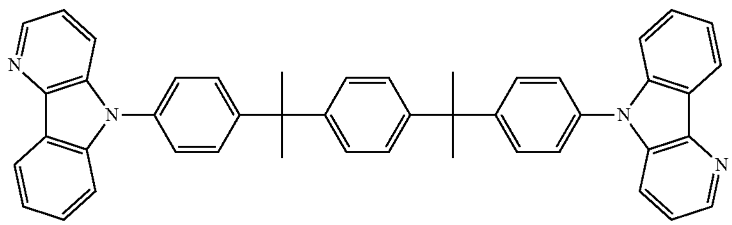
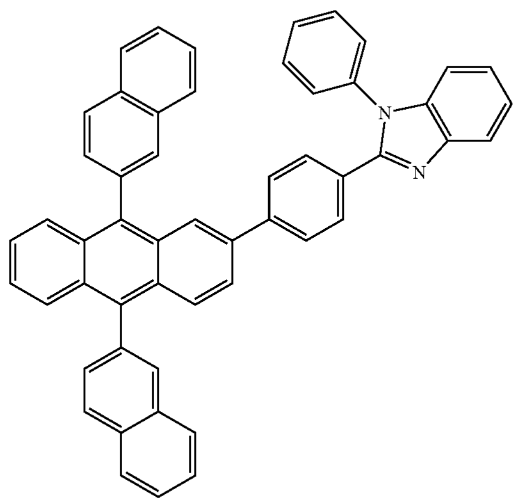
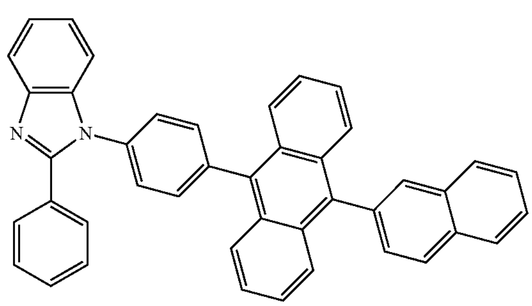
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phenothiazine-S-oxide		WO2008132085
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzoheterocycles		WO2010079051
Aza-carbazoles		US20060121308
Electron transporting materials		
Anthracene-benzoimidazole compounds		W02003060956
		US20090179554

TABLE 2-continued

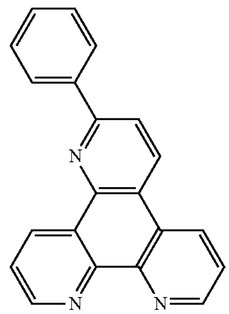
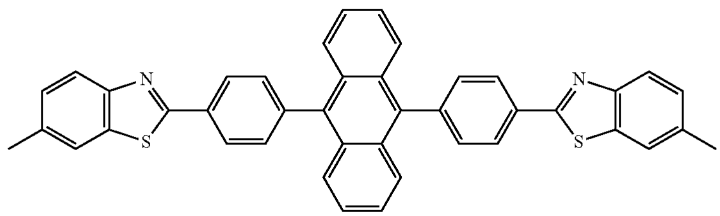
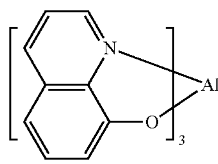
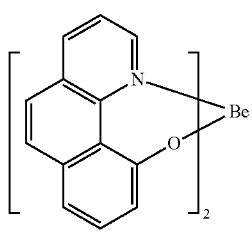
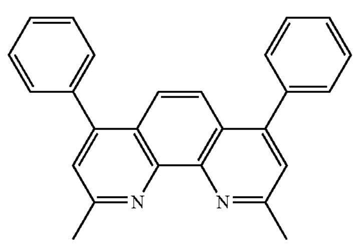
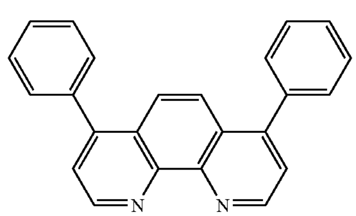
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxy-quinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) U.S. Pat. No. 7,230,107
Metal hydroxy-benoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)
		Appl. Phys. Lett. 79, 449 (2001)

TABLE 2-continued

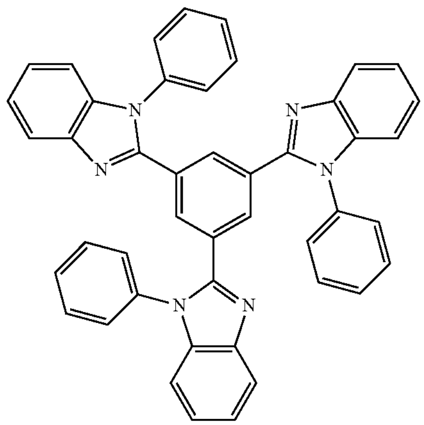
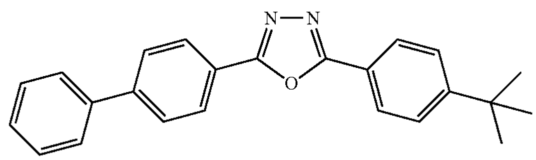
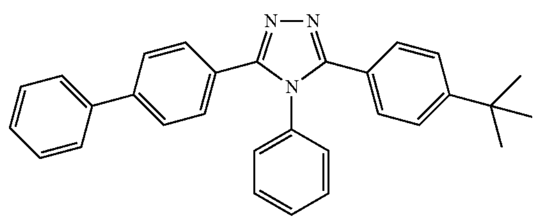
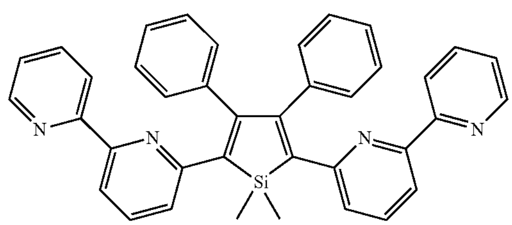
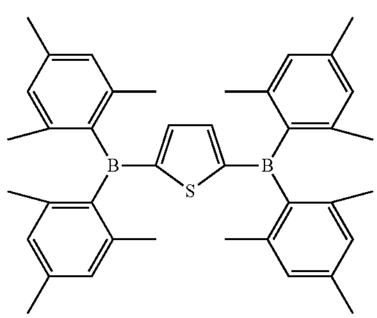
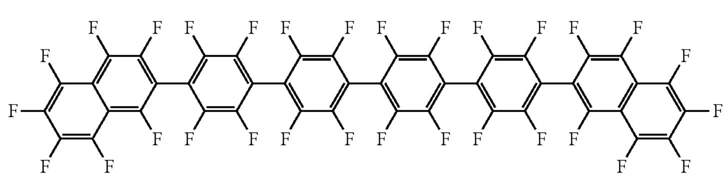
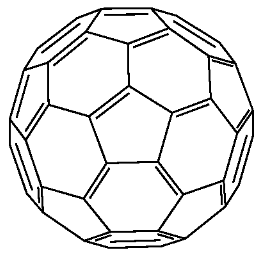
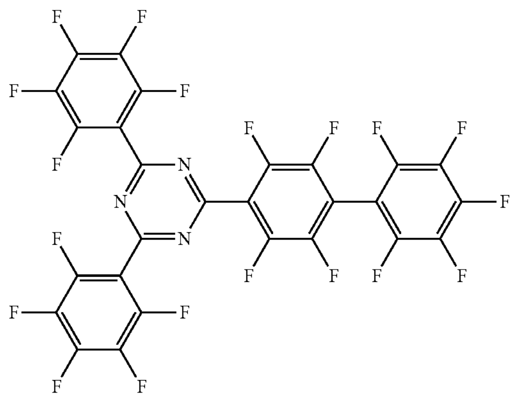
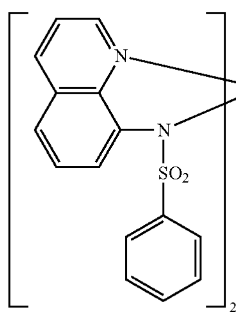
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron. 4, 113 (2003)
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)

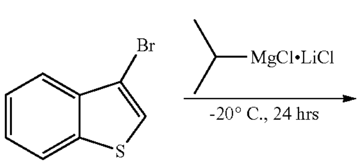
TABLE 2-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Fullerene (e.g., C60)		US20090101870
Triazine complexes		US20040036077
Zn (N^N) complexes		U.S. Pat. No. 6,528,187

EXPERIMENTAL

The intermediates described below were synthesized according to methods reported in *Angewandte. Chem. Int. Ed.* 2010, 49, 4751-4754.

Chemical abbreviations used throughout this document are as follows: Cy is cyclohexyl, dba is dibenzylideneacetone, EtOAc is ethyl acetate, DME is dimethoxyethane, dppe is 1,2-bis(diphenylphosphino)ethane, THF is tetrahydrofuran, DCM is dichloromethane, S-Phos is dicyclohexyl (2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine, Tf is trifluoromethylsulfonate.



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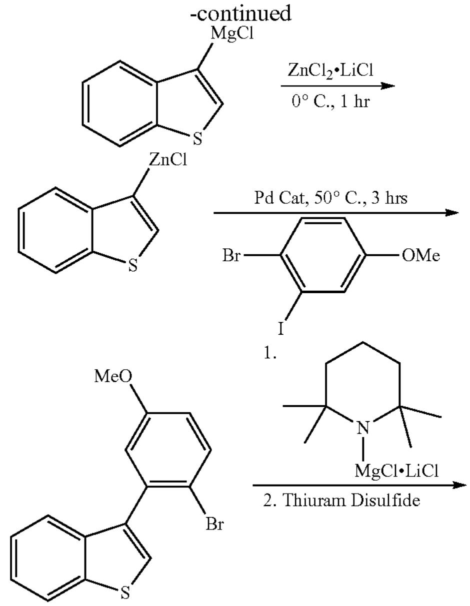

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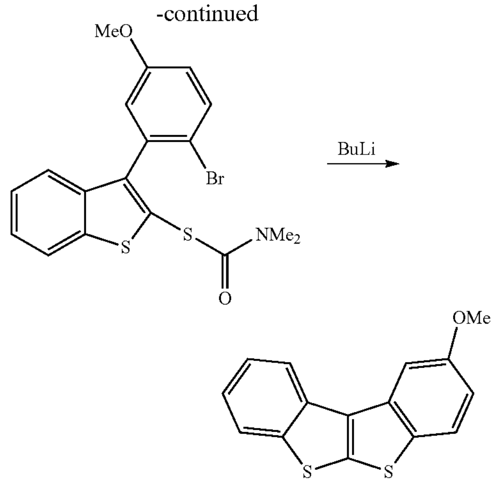
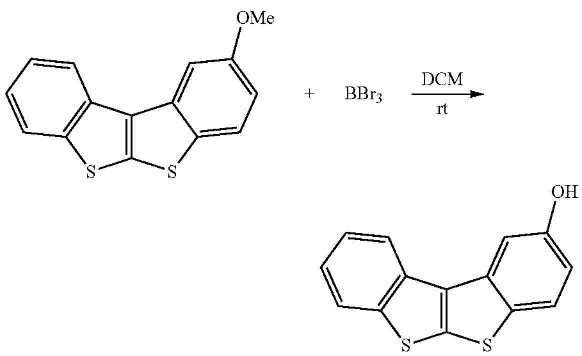
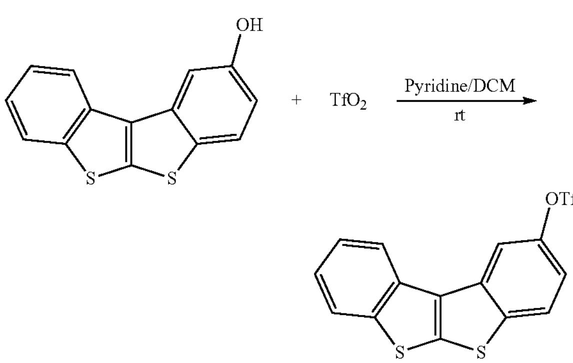


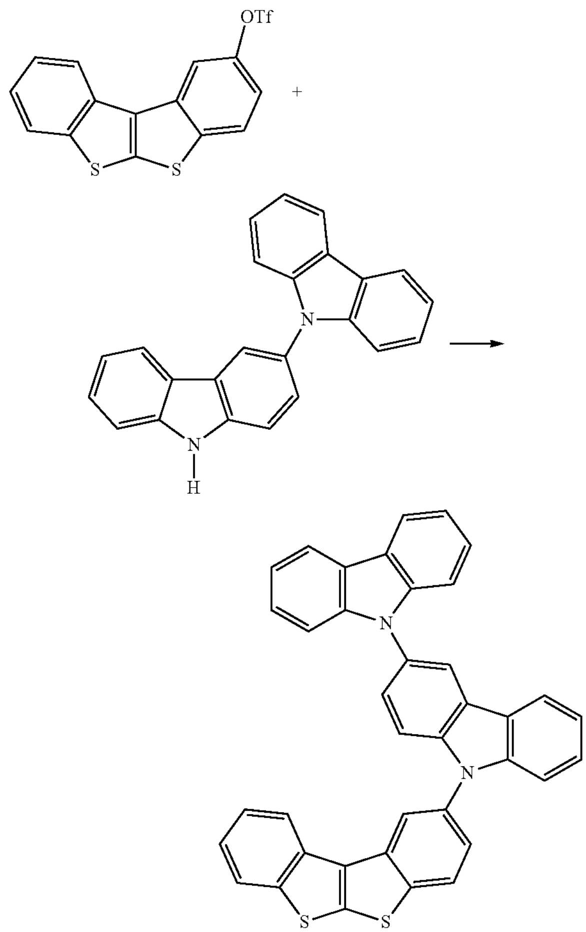
Synthesis of Compound 7



Synthesis of benzo[b]benzo[4,5]thieno[3,2-d]thiophen-2-ol. 2-Methoxy benzo[b]benzo[4,5]thieno[3,2-d]thiophen-2-ol (2.8 g, 10.36 mmol) was dissolved in 100 mL dry DCM and cooled down to −78° C., to which was added 1M BBr_3 DCM solution (15.53 mL), and the reaction was allowed to stir as the reaction was allowed to rise to room temperature. The reaction was monitored by TLC. After workup, 2.5 g (94%) of product was obtained, which was confirmed by NMR.



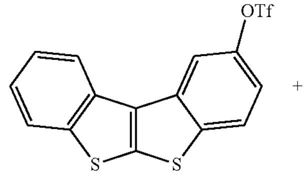
Synthesis of benzo[b]benzo[4,5]thieno[3,2-d]thiophen-2-yl trifluoromethanesulfonate. Benzo[b]benzo[4,5]thieno[3,2-d]thiophen-2-ol (2.5 g, 9.75 mmol), pyridine (3.09 g, 39 mmol) and 100 mL DCM were charged in a 250 mL flask. To this mixture, TfO_2 (13.76 g, 48.8 mmol) was added slowly and let reaction stirring at room temperature for overnight. After workup, 3 g (80%) of product was obtained, which was confirmed by GC-MS.



Synthesis of Compound 7

Benzo[b]benzo[4,5]thieno[3,2-d]thiophen-2-yl trifluoromethanesulfonate (1.2 g, 3.09 mmol), Pd2(dba)3 (0.283 g, 0.309 mmol), dicyclohexyl(2',4',6'-triisopropyl-[1,1'-biphenyl]-2-yl)phosphine (0.589 g, 1.236 mmol), 9H-3-Benzo-9'-bicarbazole (1.13 g, 3.4 mmol), sodium tert-butoxide (0.475 g, 4.94 mmol) and 50 mL of m-xylene were charged in a 100 mL flask. The mixture was bubbled with N_2 for 30 minutes then heated to reflux for 3.5 hours. The reaction was cooled down and subjected to aqueous workup. After workup, 1.2 g (68%) white solid product was obtained which was confirmed by NMR.

Synthesis of Compound 3



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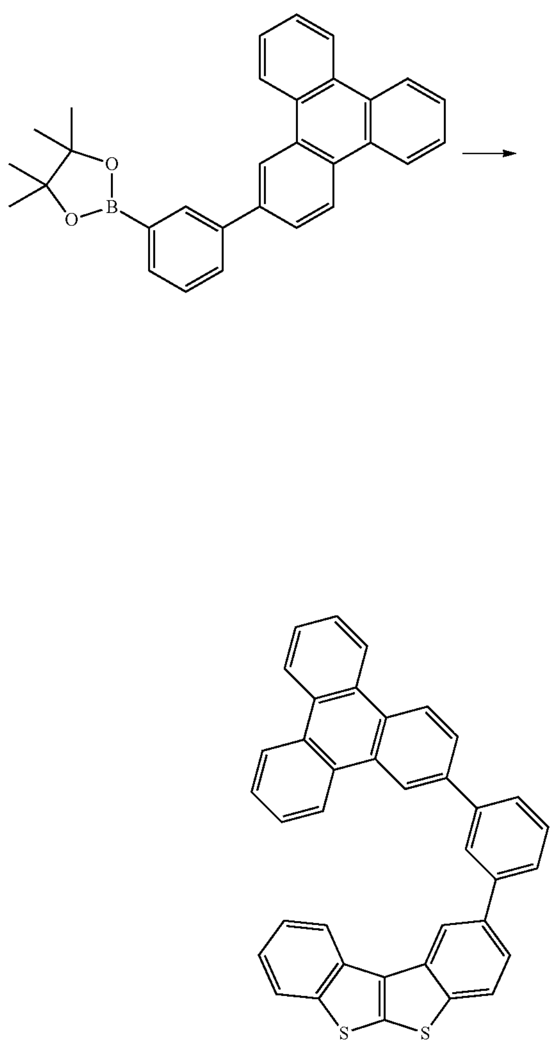
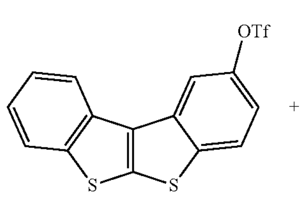


Synthesis of 2-(3-(triphenylen-2-yl)phenyl)benzo[b]benzo[4,5]thieno[3,2-d]thiophene. Benzo[b]benzo[4,5]thieno[3,2-d]thiophen-2-yl trifluoromethanesulfonate (1.5 g, 3.86 mmol), $Pd_2(dba)_3$ (0.071 g, 0.077 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.127 g, 0.309 mmol), 4,4,5,5-tetramethyl-2-(3-(triphenylen-2-yl)phenyl)-1,3,2-dioxaborolane (1.82 g, 4.25 mmol), K_3PO_4 (2.46 g, 11.59 mmol), toluene (90 mL) and water (10 mL) were charged in a 250 mL flask. This mixture was bubbling with nitrogen for 30 minutes then heated up to reflux for overnight. After purification, 1.7 g (81%) of a white solid was obtained. The compound was confirmed by NMR.

Synthesis of Compound 41



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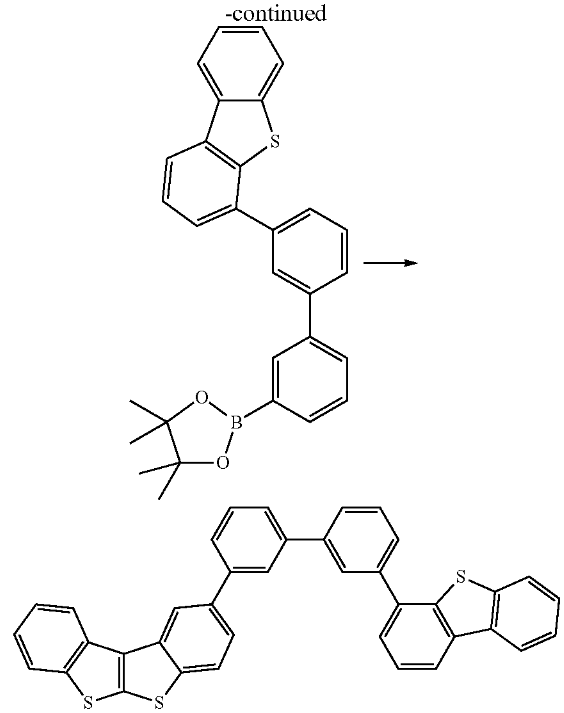
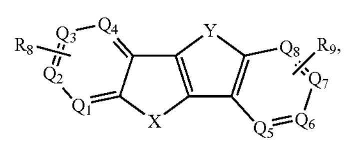


Synthesis of 2-(3'-(dibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)benzo[b]benzo[4,5]thieno[3,2-d]thiophene Benzo[b]benzo[4,5]thieno[3,2-d]thiophen-2-yl trifluoromethanesulfonate (1.3 g, 3.35 mmol), $Pd_2(dba)_3$ (0.061 g, 0.067 mmol), dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (0.11 g, 0.268 mmol), 2-(3'-(dibenzo[b,d]thiophen-4-yl)-[1,1'-biphenyl]-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1.625 g, 3.51 mmol), K_3PO_4 (2.13 g, 10.04 mmol), toluene (90 mL) and water (10 mL) were charged in a 250 mL flask. This mixture was bubbled with nitrogen for 30 minutes then heated to reflux overnight. After purification, 1.5 g (78%) of a white solid was obtained. The compound was confirmed by NMR.

It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

The invention claimed is:

1. A compound having the formula:



wherein Q_1 to Q_8 are independently selected from C and N, and wherein Q_1 to Q_8 may be further substituted;

wherein X and Y are independently selected from the group consisting of O, S, and Se;

wherein R_8 and R_9 independently represent mono, di, tri, tetra substitution, or no substitution;

wherein R_8 and R_9 are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof;

wherein at least one of R_8 and R_9 is not hydrogen or deuterium; and

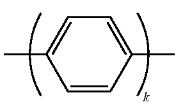
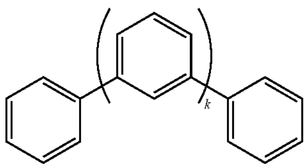
wherein at least one of the following is true:

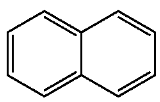
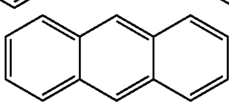
(1) one or more of Q_1 to Q_8 is N;

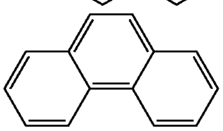
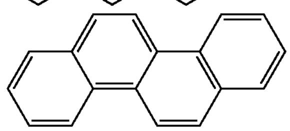
(2) Q_2 is C substituted by R_{8-2}, which is hydrogen, and Q_7 is C substituted by R_{9-7}, which is hydrogen; and

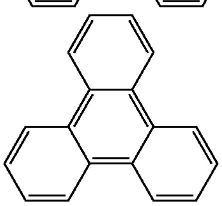
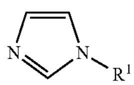
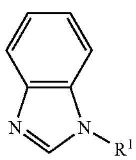
(3) each R_8 is hydrogen or deuterium.

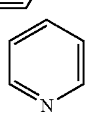
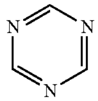
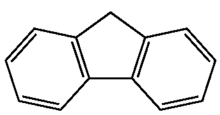
2. The compound of claim **1**, wherein at least one of R_8 and R_9 is independently selected from the group consisting of:

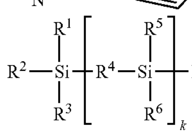
, ,

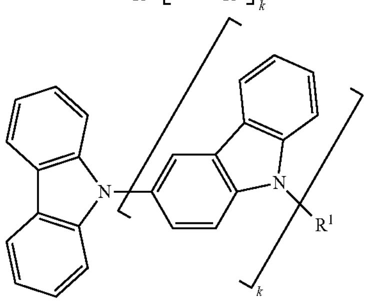
, ,

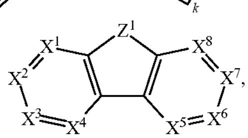
, ,

, , ,

, , ,



,



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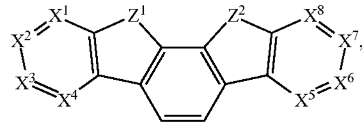
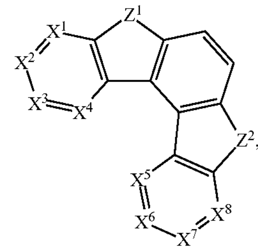
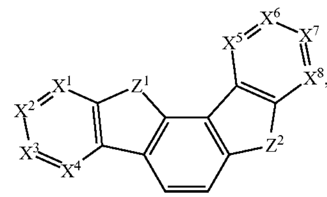
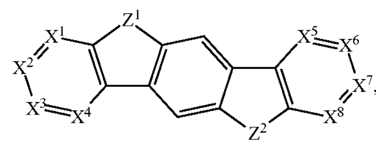
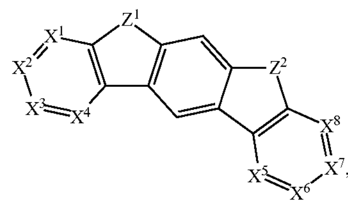










wherein R^1 to R^7 is independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof;

wherein k is an integer from 0 to 20;

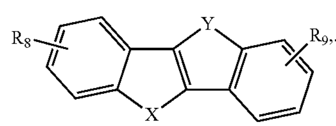
wherein X^1 to X^8 are independently selected from C, CH, and N;

wherein Z^1 and Z^2 is selected from NR^1, O, or S; and

wherein R_8 and R_9 may be further substituted.

3. The compound of claim **1**, wherein the compound has the formula:

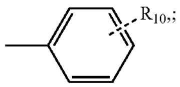
Formula III



4. The compound of claim **1**, wherein one of Q_1 to Q_8 is N.

5. The compound of claim **1**, wherein at least one of R_8 and R_9 has the formula:

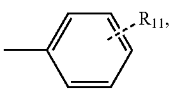
Formula IV

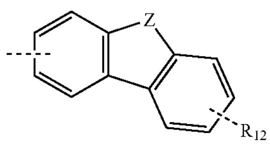


wherein R_{10} represents mono, di, tri, tetra substitution, or no substitution; and

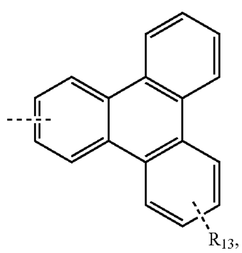
wherein R_{10} is selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

6. The compound of claim 5, wherein R_{10} represents mono-substitution and is selected from the group consisting of:





,



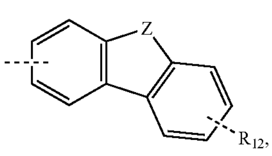
SiRR'R" and combinations thereof;

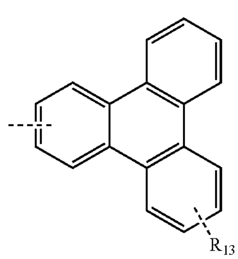
wherein Z is selected from the group consisting of NR, S, O, and Se;

wherein R_{11}, R_{12}, and R_{13} represents mono, di, tri, tetra substitution, or no substitution; and

wherein R, R', R", R_{11}, R_{12}, and R_{13} are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

7. The compound of claim 1, wherein at least one of R_8 and R_9 is independently selected from the group consisting of:





,

SiRR'R" and combinations thereof;

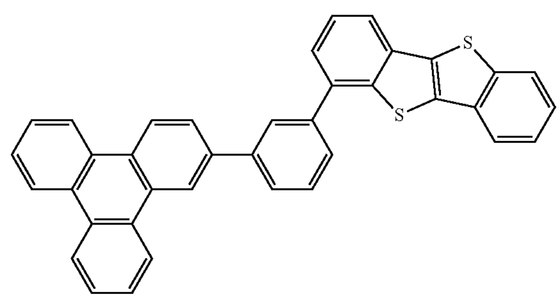
wherein Z is selected from the group consisting of NR, S, O, and Se;

wherein R, R', R", R_{12}, and R_{13} are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof.

8. The compound of claim 1, wherein each R_8 is hydrogen or deuterium.

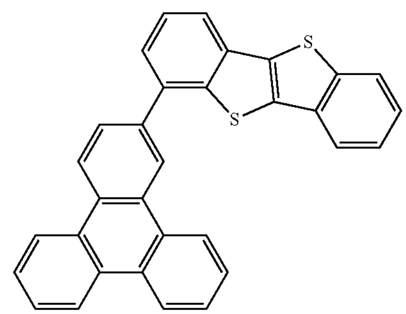
9. The compound of claim 1, wherein the compound is selected from the group consisting of:

Compound 31



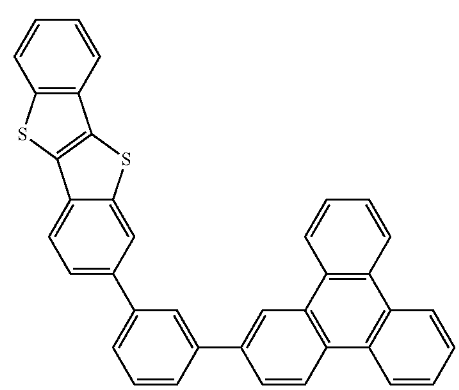
,

Compound 32



,

Compound 45



, and

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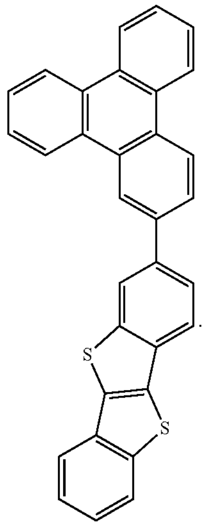
Compound 46



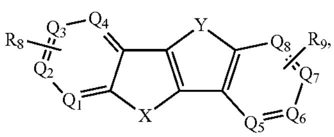
10. A first device comprising an organic light emitting device, further comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound having the formula:

Formula III



wherein Q_1 to Q_8 are independently selected from C and N, and wherein Q_1 to Q_8 may be further substituted;

wherein X and Y are independently selected from the group consisting of O, S, and Se;

wherein R_8 and R_9 independently represent mono, di, tri, tetra substitution, or no substitution;

wherein R_8 and R_9 are independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, arylalkyl, amino, silyl, germyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combinations thereof;

wherein at least one of R_8 and R_9 is not hydrogen or deuterium; and

wherein at least one of the following is true:

(1) one or more of Q_1 to Q_8 is N;

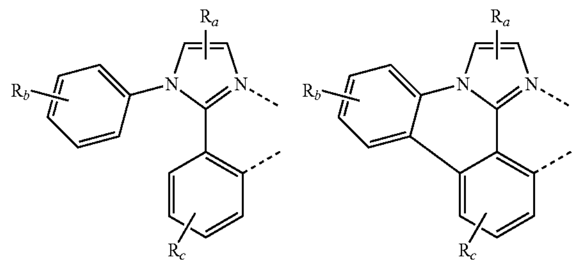
(2) Q_2 is C substituted by R_{8-2}, which is hydrogen, and Q_7 is C substituted by R_{9-7}, which is hydrogen; and

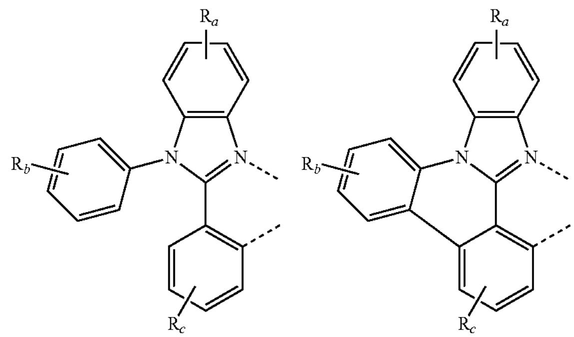
(3) each R_8 is hydrogen or deuterium.

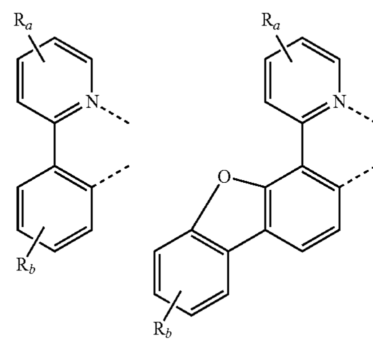
11. The first device of claim 10, wherein the organic layer is an emissive layer and the compound of Formula III is a host.

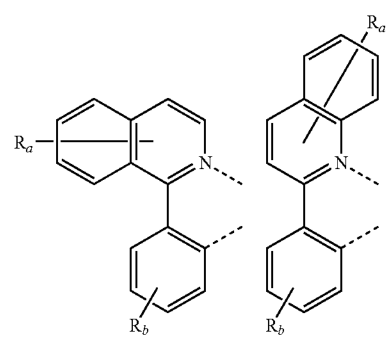
12. The first device of claim 10, wherein the organic layer further comprises an emissive dopant.

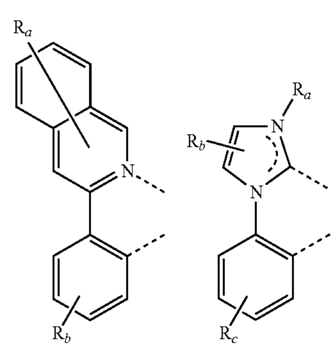
13. The first device of claim 10, wherein the emissive dopant is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:











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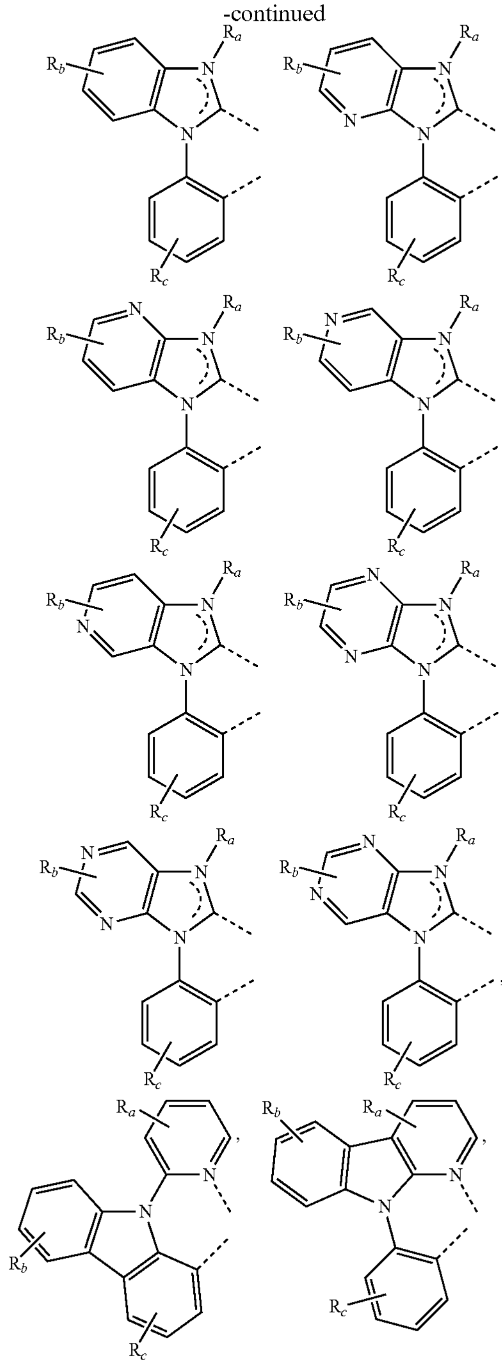

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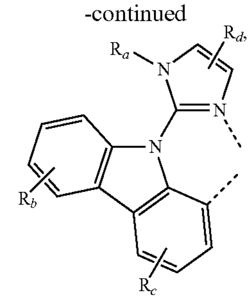

wherein R_a, R_b, and R_c may represent mono, di, tri, or tetra substitution, or no substitution;

wherein R_a, R_b, and R_c are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein two adjacent substituents of R_a, R_b, and R_c are optionally joined to form a fused ring or form a multidentate ligand.

14. The first device of claim **10**, wherein the device further comprises a second organic layer that is a non-emissive layer and the compound having Formula I is a material in the second organic layer.

15. The first device of claim **14**, wherein the second organic layer is a blocking layer and the compound having Formula I is a blocking material in the second organic layer.

16. The first device of claim **10**, wherein the first device is a consumer product.

17. The first device of claim **10**, wherein the first device is an organic light-emitting device.

18. The first device of claim **10**, wherein the first device comprises a lighting panel.

19. The compound of claim **1**, wherein Q_2 is C substituted by R_{8-2}, which is hydrogen; and Q_7 is C substituted by R_{9-7}, which is hydrogen.

20. The compound of claim **1**, wherein one or more of Q_1 to Q_8 is N.

* * * * *